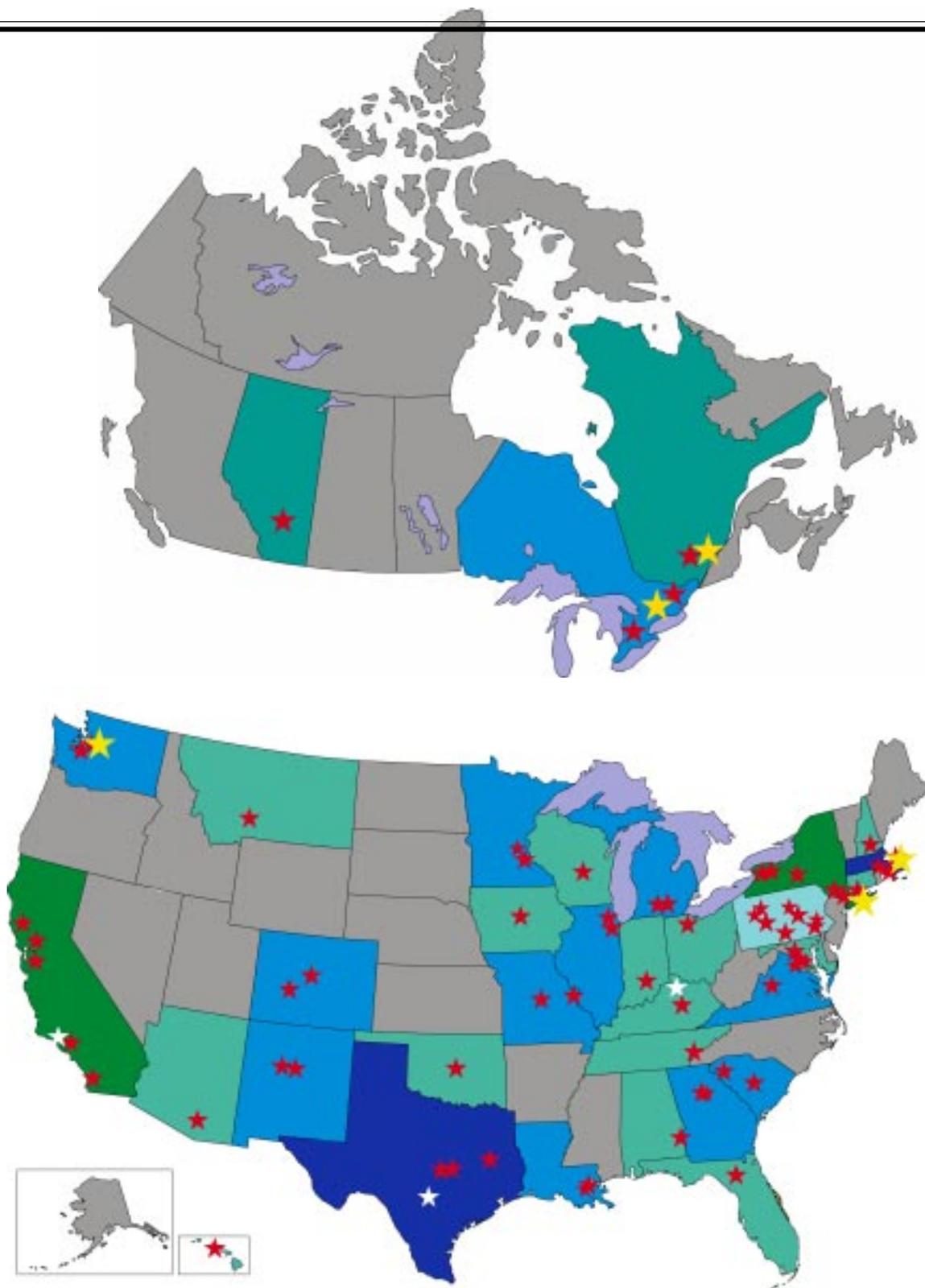


AMERICAN CRYSTALLOGRAPHIC  
ASSOCIATION

# NEWSLETTER

Number 2

Summer 2000



*The ACA at 50 - With Lots of Room to Grow*

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

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**President's Column**



The thought that we could use the ACA website to better advantage to improve education has prompted me to try to get a website upgrade project underway. We need to educate those who lack formal training but have become interested in some aspect of crystallography. Some will need to know practical things: how to avoid pitfalls, etc. because their primary need is to do a crystal structure.

Some may want to follow their noses to learn more about theory: symmetry principles; Fourier transforms; diffraction physics, etc. Some of the education might be aimed at the high school level, but there should be good opportunities for the more advanced student. On a different track, we also need to educate practicing crystallographers about new software, new instruments, new resources and new technology, the tools of our trade. Many of us are so busy that the hurdle of learning to use a software tool that is new (or new to us) may well prevent us from trying it out. The ACA website already has some good links. Last year Virginia Pett and Kathy Kantardjjeff compiled a list of links to crystallographic education sites; there are a number of other useful links in place; and there is a good brochure aimed at high school students. Nevertheless, we have barely scratched the surface of what could be done. Since this is not a job that Marcia Evans or Sally Lunge in the Buffalo office should be asked to tackle, I suggested the idea to Doug Rees (Publications- soon-to-become-Communications Committee chair) and Bob Von Dreele (Crystal Data & Computing Committee chair) and they both responded with enthusiasm. I asked them, together with their committee members, to exchange ideas about ways and means. Since there is so much on the web already, much can be done just with structuring and describing appropriate links, but there may also be clear needs for development of particular topics not on any other sites. Bob Von Dreele attended the March Council meeting, and suggested that the actual work of developing the website might be best accomplished by students as a graduate research project. The Council is amenable to the idea of funding such a project and we certainly encourage anyone interested to submit a proposal. We would also be grateful for suggestions and particularly grateful for any offers of help.

The 50<sup>th</sup> anniversary of ACA has also been much on my mind. All past presidents of ACA received special invitations to attend the St. Paul meeting and the Wednesday

evening banquet, and they were also invited to write about their recollections of the ACA. The correspondence this has elicited has been great fun, and I have enjoyed reading all the memoirs. These are being collected and will be printed, together with any photos that can be gathered, in booklet form. Much of the material appears in this newsletter as well. For the rest of this year, the newsletter will continue to publish articles and photos related to our history, so please do search your memories and your photo albums and submit interesting material to Judy Flippen-Anderson or Ron Stenkamp.

Also with ACA history in mind, Council has decided that we need a committee that could provide a vision of what we should be doing to ensure that we keep track of the ideas and the things that have contributed significantly to our scientific development. Jenny Glusker agreed to chair this committee, and Hugo Steinfink and Bryan Craven are the other members. Please let them know any thoughts you have along these lines.

The St. Paul meeting is coming up soon. If you plan to attend, I hope you will not miss the opening reception in the new science museum because this promises to be one of our best ever parties. The YSIG mixer at a nearby pub also has great potential for pleasurable ambience, as does the 50<sup>th</sup> anniversary river cruise. See you in St. Paul!

*Connie Chidester*

### *Council News*

The ACA Council met for ca. 9 hours on Saturday March 18<sup>th</sup> at the HWI in Buffalo. Plans for the annual meeting in St. Paul are in place. In addition to the *Transactions Symposium* there will be a symposium featuring HHMI investigators, organized by and now dedicated to Paul Sigler. Awards presentations for the Warren Award to Ian Robinson and the Buerger Award to Lyle Jensen will also take place. Invitations to attend the meeting have been sent out to the 34 living past presidents of the ACA.

The ACA is in good financial health, but membership has been approximately constant for the past few years. There were discussions of budgetary issues, ACA publications, improving the publicity of ACA awards, and initiation of a History/Archives Committee for the ACA. Some time was spent discussing how the ACA web site might be improved. Future meeting sites were discussed, particularly the 2003 in Cincinnati/Northern Kentucky and the possibility of returning to Canada for the 2004 meeting.

The ACA is now sending representatives to AAAS meetings to represent the ACA on a variety of subcommittees. Canadian Rep. Louis Delbaere reported on activities in Canada, including the new Synchrotron being built in Saskatchewan and increases in funding expected for biomedical research. Outreach to Central and South American crystallographers and how they might interact with or participate in the ACA was discussed.

In due course the minutes of the meeting will be posted on the web. Minutes of previous Council Meetings can be found at <http://www.hwi.buffalo.edu/ACA/Society-Info/council-reports.html>

*Lee Brammer*

### *Small Angle Scattering SIG: Neutron Focusing with Compound Refractive Optics Demonstrated at the NIST Center for Neutron Research*

Since refractive indices for cold neutrons (wavelength ~ 1nm) differ from unity by at most a few parts in 100 thousand, grazing incidence reflection optics have long been considered the most promising means for focusing neutrons for applications such as small-angle neutron scattering (SANS). Numerous attempts over more than 30 years to produce reflective surfaces for neutrons have been vitiated, however, by SANS from the mirror surfaces themselves, which blurs the focus. The best mirrors produced thus far are only marginally better for SANS than pinhole collimation, i.e., simple apertures separated by long distances.

Scientists at Bell Laboratories [M. R. Eskildsen, P. L. Gammel, E. D. Isaacs, C. Detlets, K. Mortensen, D. J. Bishop, *Nature* **391**, 563-566 (1998)] recently took a fresh look at this problem and proposed that multiple refraction from high index, low absorbing material could be superior to reflection optics or conventional pinhole collimation for SANS. Measurements made recently at NIST's Center for Neutron Research (NCNR) in collaboration with the Bell Labs scientists have demonstrated that this is indeed the case [S.-M. Choi, J. G. Barker, C. J. Glinka, Y. T. Cheng, P. L. Gammel, *J. Appl. Cryst.* (in press, 1999)]. Using a linear array of 28 biconcave magnesium fluoride lenses, a beam of 0.85 nm neutrons, from a source aperture 15 m from the lenses, was focused onto a detector 15 m away. Most importantly, parasitic scattering from the lenses was 10,000 times less than the peak intensity, a marked improvement over reflection optics.

The focusing lenses are now installed for routine use in one of the NCNR's 30-meter SANS instruments. Experiments on polymer composites and high  $T_c$  superconductors, for example, using the focusing lens system, have demonstrated more than an order of magnitude improvement in sensitivity to structural features, 50% larger than had been possible at the NCNR with pinhole collimation.

*Tom Reiker*

### *Small Molecule SIG: The SIG Web Page has Moved*

The Small Molecule SIG Web Page is now at:

[http://www.iumsc.indiana.edu/sm\\_sig/index.html](http://www.iumsc.indiana.edu/sm_sig/index.html)

Comments and suggestions about this webpage should be addressed to:

John Bollinger the new Small Molecule SIG Webmeister at [jobollin@indiana.edu](mailto:jobollin@indiana.edu)

**Request for Nominations  
Elizabeth A. Wood Award**

The ACA Science Writing Award has been named in honor of Elizabeth Armstrong Wood for the breadth and clarity of her writing. It is intended to honor people who have written books or articles that bring science, especially crystallography or the results of crystallographic studies, to the attention of a wider audience. Successful nominees need not be crystallographers or scientists, and 'writing' could include artistic efforts, museum displays, etc.

Previous winners include Roald Hoffmann of Cornell, Robert Hazen of the Carnegie Institution in Washington, DC and Robert A. Weinberg of MIT.

Nominations should include the titles of books, copies of articles, or other documentation and should be submitted to the ACA office. Selection of the winner will be made by ACA Council.

**Update on the Canadian Light Source**

Construction began on the Canadian Light Source (CLS) in Saskatoon, Canada in July 1999 on the University of Saskatchewan campus. The six-story, stadium-sized building that will house the CLS will be built by December 2000, and the \$173.5 million (Cdn) facility should be operational by January 2004. Most of the framework steel has now been erected (1300 tons, with 8 roof trusses that span 84 meters and weigh 67 tons each). More than \$37M (Cdn) in contracts have been let already for nearly all of the building, the booster ring and the dipole magnets of the main ring. The project remains on schedule and on budget. Photos of the construction are available on the website address [http://cls.usask.ca/Site\\_photos/index.html](http://cls.usask.ca/Site_photos/index.html)

Louis Delbaere

**IMPORTANT NOTICE for  
ACA 2000**

**Due to problems with the  
registration form the hotel could  
not decipher some reservations.  
Please check directly with the  
hotel to be sure that your  
reservation is in order.**

**(651) 292-1900**

**ACA Members Selected for  
Prestigious Awards**

Helen M. Berman (Rutgers) was named an Outstanding Woman Scientist by the New York Chapter of AWIS (American Women in Science).

David S. Eisenberg (University of California, Los Angeles) received the Repligen Award, given by the American Chemical Society, for his work on the relationship of protein sequence to three-dimensional structure and function.

Brian W. Matthews (U. of Oregon and Howard Hughes Medical Institute) will receive the Stein and Moore Award from the Protein Society for his pioneering contributions to X-ray crystallographic methods, protease structure, gene regulation and mutational analysis of protein stability.

**NIST Centennial Celebration -  
Crystallographic Highlights**

Year 2001 is the Centennial celebration of the National Institute of Standards and Technology (NIST), formerly known as the Bureau of Standards (NBS). NIST has a long history of crystallographic research, and has made significant contributions to the advancement of the field of crystallography. In the winter issue of the ACA newsletter, a feature article about the historical and current research interests of crystallography at NIST will be published as a result of the combined efforts of NIST crystallographers and collaborators from various disciplines. Examples of areas to be highlighted include:

- Early history* (H. McMurdie)
- High pressure crystallography* (G. Piermarini)
- Origins of accuracy in structural measurements* (R. Deslattes)
- Neutron diffraction* (A. Santoro)
- Quasi-crystals* (E. Prince, J. Cahn, and D. Shechtman)
- International Tables for Crystallography* (E. Prince)
- Synchrotron science* (G. Long)
- Standard x-ray powder diffraction patterns* (H. McMurdie and W. Wong-Ng)
- Crystal Data* (V. Karen)
- Crystallography of Portland cement* (P.

- Stutzman)
- Crystallography of dental materials* (M. Mathew)
- Protein crystallography and Protein Data Bank* (T. Gallagher, T.N. Bhat, and G. Gilliland)
- Standard ref. materials for powder diffraction* (J. Cline)
- Electron diffraction* (L. Bendersky)
- Polymer crystallography* (J. Barnes)
- Single crystal structural studies* (A. Mighell and W. Wong-Ng)
- Standard reference material for single crystal diffractometer* (W. Wong-Ng, T. Siegrist, G. DeTitta, and L. Finger)
- Phase equilibria diagrams* (H. McMurdie and H. Ondik)

For more detailed information, please contact the co-editors of the article (Winnie Wong-Ng, phone: 301-975-5791, e-mail: [winnie.wong-ng@nist.gov](mailto:winnie.wong-ng@nist.gov); or Alan Mighell, phone: 301-975-6254, e-mail: [alan.mighell@nist.gov](mailto:alan.mighell@nist.gov))

**Both Seattle and  
Cambridge (MA) have  
hosted the ACA and the  
IUCr but only Harvard has  
been the home to both.  
Pittsburgh has hosted 3  
ACA meetings, 2 at  
Carnegie Mellon and 1 at  
Pitt. ACA has met twice at  
the University of  
Washington and at UT  
Austin.**

We gratefully acknowledge the continued support of

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## INTERNATIONAL CENTRE FOR DIFFRACTION DATA

### Ludo Frevel Crystallography Scholarship Awards

The science of crystallography has played a key role in the development of X-ray diffraction, electron diffraction, and neutron diffraction for the elucidation of the atomic structure of matter. Crystallography is an interdisciplinary branch of science taught in departments of physics, chemistry, geology, molecular biology, metallurgy, and materials science. To encourage promising graduate students to pursue crystallographically-oriented research, the International Centre for Diffraction Data (ICDD) has established the Crystallography Scholarship Fund. Now known as the Ludo Frevel Crystallography Scholarship Fund, its new name was recently adopted to honor the founder of the fund, Dr. Ludo Frevel. While the Ewald Prize is awarded every three years to an internationally recognized crystallographer, little effort has been made by science departments to cultivate aspiring crystallographers. Convinced of the beneficial scientific impact of the proposed scholarships for crystallographically-oriented research, the ICDD has solicited funds from private and industrial sectors to support this program. The ICDD has awarded 33 scholarships since 1992. The year 2000 Scholarship Awards were in the amount of \$2,250 each. Applications for the year 2001 awards must be received by the ICDD no later than 31 October 2000.

**Qualifications :** The applicant should be a graduate student seeking a degree with major interest in crystallography e.g. crystal structure analysis, crystal morphology, modulated structures, correlation of atomic structure with physical properties, systematic classification of crystal structures, phase identification and materials characterization. There are no restrictions on country, race, age or sex. The term of the scholarship is one year. Application for one renewal may be made by the recipient at the end of the first year. Because a limited number of scholarships are awarded, renewal applications will be considered on a competitive basis in conjunction with all applications that have been submitted up to the closing date.

**Submit:** Curriculum Vitae, listing degree(s) held and degree(s) sought. A one-page proposal by the graduate student describing the type of crystallographic research to be partially supported by scholarship. A supportive letter from the sponsoring professor of an accredited university or an institute of technology on institution letterhead.

**Restrictions on the scholarship fund:** The scholarship stipend is to be used by the graduate student to help defray tuition and laboratory fees. A portion of the stipend may be applied to registration fees to accredited scientific meetings related to crystallography. No more than one scholarship will be awarded to applicants at any one accredited institution per year. The funds of the scholarship are not to be used for travel.

The awarding of the scholarships is administered by a committee consisting the ICDD Scholarship Committee Chairman, the ICDD Chairman and Past Chairman, the Chairman of the ICDD Education Subcommittee, the ICDD Executive Director, and three individuals without conflict of interest. One or more accredited professors (with no conflicts of interest) may be invited to assist in the selection of successful candidates.

Applications must be received by 31 October 2000. Please mail to: Scholarship Awards Committee c/o Secretary, ICDD, 12 Campus Boulevard, Newtown Square, PA 19073-3273 U.S.A.

### George A. Jeffrey (1915-2000)

Professor George Jeffrey (known as Jeff) died at his home in Pittsburgh on February 13. At 84 years old, Jeff was enjoying a full life but he contracted amyotrophic lateral sclerosis (Lou Gehrig's disease) which progressed rapidly.

As a structural crystallographer, Jeff was widely known for his studies of hydrogen bonds. These provide the weak attractions that hold together biological molecules ranging from water to DNA and proteins. Jeff specialized in determining the molecular arrangement and hydrogen bonding in crystals of carbohydrates and in crystals where water molecules form cages to trap other molecules. He was the author of two books on hydrogen bonds and also more than 300 research articles. In the early '50s, Jeff became a pioneer in the use of digital computers for X-ray crystal structure analysis. At a time when his laborious computations involved slide-rules and cash registers that added in pounds, shillings and pence, Jeff foresaw the importance of the digital computers which now make possible the crystal structure determination of the giant molecules necessary for life.

George Jeffrey was born in Cardiff in Wales and was educated in England. He received his Ph.D. in Chemistry from the University of Birmingham in 1939 and a D.Sc. in 1953. His Ph.D. thesis was on the crystal structure of salts of the carbohydrate glucosamine. During the war, he was a research physicist at the British Rubber Producers Research Association. There he worked out the crystal structure of geranylamine hydrochloride, which contains a subunit of rubber. These early organic structures were among the first to be analysed by three-dimensional X-ray crystallography. After a Lectureship at the University of Leeds, Jeff came to the University of Pittsburgh, Pennsylvania, first as a visiting professor and then to stay, in 1953. He remained at Pitt until his retirement in 1985, except for two years (1974-6) at the Brookhaven National Laboratory. Until 1966, he held a full professorship in the Departments of Physics, Chemistry and Earth and Planetary Science. Then he was honored with the shorter title, University Professor. After 1985, he remained active as University Professor Emeritus.

Jeff rapidly built up the Crystallography Laboratory at Pitt and was soon attracting students, postdoctoral fellows and visiting professors from all over the world. Formal evening classes in X-ray crystallography were attended by his research group and also by scientists from the many corporate research laboratories in the Pittsburgh area. Jeff's success depended not only on scientific excellence but also on his ability to make his co-workers feel like members of his crystallographic family. Jeff and Maureen made them all welcome at their home. Jeff was a strong leader. The sign on his desk said "Be reasonable, do it my way." Jeff's style was to develop a logical plan and then to back it by his powers of persuasion. Invariably, his way

seemed to be the right way. In 1969, he persuaded the University to establish Crystallography as a graduate department, the only one of its kind in the U. S. At most times there were about 40 members, including up to 5 tenure-stream faculty and 15 students. Adjunct faculty appointments linked the Crystallography Department with other research groups, notably the Biocrystallography Laboratory at the nearby V. A. Medical Center. Eventually, 76 students obtained their Ph.D. in Crystallography and another 7 obtained their M. S.

Jeff was President of the American Crystallographic Association in 1963 and Co-editor of *Acta Crystallographica* (1973-84). He took every opportunity to travel in the U.S. and abroad. He was an American Chemical Society Tour Speaker (1964, 1969 and 1974), Robert Welch Foundation Lecturer (1979), UNESCO advisor to Pakistan (1967), visiting professor at the University of Sao Paulo (1970), Senior Fulbright Scholar in Portugal (1973), Hassel Lecturer in Norway (1975), Alexander von Humboldt U.S. Senior Scientist Awardee in Germany (1983) and Director of NATO Advanced Study Institutes in Portugal (1987) and Spain (1990).

Among his awards, Jeff received the Hudson Award of the American Chemical Society (1980), the Buerger Award of the American Crystallographic Association, and the Haworth Award of the Royal Society of Chemistry of the United Kingdom (1998).

*Bryan Craven*

### *An Award in Memory of George A. Jeffrey*

Jeff was well known and will be missed by many chemists and crystallographers around the world and especially by his saddened colleagues and former students at the University of Pittsburgh. In order that memories of him will live on, it is intended to set up the Jeffrey Award. Jeffrey Awards will provide funds for graduate students to attend the triennial Congress of the International Union of Crystallography. Applications will be invited world-wide from students who have outstanding research results to present at the Congress. Jeff's family and friends believe that he would be greatly pleased to be remembered in this way.

The Jeffrey Award will be administered by the Pittsburgh Diffraction Society which is incorporated as a not-for-profit organization. Please send donations in U. S. currency to Dr Bryan Craven, Chemistry Department, Indiana University of Pennsylvania, Indiana, PA 15705. Checks should be made out to "The Jeffrey Fund/Pittsburgh Diffraction Society". These donations will be U. S. tax-deductible.

*Bryan Craven, President, Pittsburgh Diffraction Society*

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### *Joshua Ladell (1923 - 2000)*

Joshua Ladell passed away in Jerusalem, Israel, on January 28, 2000 after a lengthy illness. Josh was born in New York City May 19, 1923. He served in the US army from 1943 to 1946 and after his discharge continued his studies at Brooklyn College where he received the B. A. degree in 1948. He pursued graduate studies in Physics at the Polytechnic Institute of Brooklyn (now the Polytechnic University of New York) where he received the M. S. degree in 1951 and the Ph. D. in 1954. His dissertation was done under the supervision of the eminent crystallographer Professor I. Fankuchen. Among the graduate students Josh was the first to attempt a least squares crystal structure refinement using the inchoate computation facilities at the IBM Watson Laboratory. He commuted from Poly to the Watson laboratory for one summer and although we can't recall the result it was a very stimulating experience for him that he shared with the other graduate students. Josh was always generous with his time to discuss and help other graduate students, and later colleagues, with their research. He established excellent relationships with the faculty that blossomed into friendships after his graduation.

After receiving his Ph.D Josh was awarded a Lipsky exchange fellowship that enabled him to spend 1954 - 1956 with Gerhardt Schmidt at the Weizmann Institute of Science in Rehovot, Israel. During his stay in Israel he was recruited by William Parrish to join the Philips Laboratories in Irvington and Briarcliff Manor, New York upon his return to the US. Initially he was in the powerful x-ray research group headed by Bill Parrish, and ultimately led the x-ray research efforts of that group. His work there included studies of the geometrical optics of single crystal diffractometers, applications of crystallography to fluorescence analysis instrumentation, the theory of instrumental diffraction profiles, the development of the PAILRED automated single crystal diffractometer system in 1966, the use of dedicated microprocessors to control x-ray diffraction instruments, and the use of forbidden reflections to solve the phase problem. He developed a generalized powder diffractometer, which also could take account of preferred orientation in polycrystalline samples and enabled texture and pole figure studies. He and two coworkers published two seminal papers on the determination of surface state electronic density in thermally oxidized silicon that is frequently cited in most technology textbooks. He presented his research at numerous ACA meetings, published approximately 50 papers in technical journals and was awarded several patents.

A few years after his retirement from Philips in 1991 he and his wife Bea decided to follow one of their sons and his family, who had settled in Israel, and moved to Jerusalem. His wife continues to reside there. Josh was a dedicated scientist-crystallographer, friend and colleague. He will be sorely missed by all who knew him.

*Hugo Steinfink, Nathan Spielberg*

### ORTEP of the Year Award

The R. Harlow Foundation for Disabused Crystallographers will, as usual, be presenting a check for \$200 at the St. Paul ACA Meeting this summer for the best example of how an ORTEP drawing was used to spot and resolve a "problem" structure. Any published structure in a refereed journal is eligible for submission, but the submitter must clearly demonstrate the manner in which ORTEP (or more generally, any thermal-ellipsoid plotting program) was used to indicate that the structure as published was incorrect and must provide an ORTEP of the "corrected" structure. Structure determinations where the ORTEP drawing failed to indicate a "problem" structure are also eligible; these too are educational. Entries should be addressed to the Foundation at 7 Shull Dr., Newark, DE, 19711, USA. You do not have to be present at the Meeting to win. Since this award is made on a continuing basis submissions received too late to be considered for the Y2K award will automatically be considered for the 2001 contest.

I would also like to point out to the crystallographic community two other Foundation initiatives, the Hydrogen Challenge and the Low-Temperature Prize. Details of these awards can be found under the ACA Service SIG web page at <http://www.pitt.edu/~geib/aca.html>. In addition, I am looking for examples of misprinted stereo ORTEPs. i.e. stereo pairs reversed, same image twice (no stereo effect), etc. For entries in this category, I will send you a small token of my appreciation.

*R. Harlow*

### New ICDD/NIST Cooperation

The International Centre for Diffraction Data ([www.icdd.com](http://www.icdd.com)) is pleased to announce a new area of cooperation with the National Institute of Standards and Technology. There has been a long history of productive cooperation between these two organizations, and the new initiative extends this cooperation to allow the interchange of crystallographic data from metallic substances. While there are about 25,000 experimental metal and alloy patterns already in the PDF, there are also several thousand additional alloys where only single crystal data are available. These materials are not represented in either the PDF or the NIST Crystal Data File. The new cooperative agreement aims to gather, and critically edit these data, then to calculate the powder patterns and use these data to fill the gaps in the PDF. Similar agreements are already in place with the CCDC that maintains the Cambridge Structure Database and FIZ that maintains the Inorganic Crystal Structure Database. The size of the PDF has more than doubled in the past 3 years, as a result of these agreements, and with expansion of the ICDD Grant-in-Aid program. The new agreement with NIST should further enhance the PDF by providing comprehensive coverage for metals and alloys.

*Helen M. McDonnell ([mcdonnell@icdd.com](mailto:mcdonnell@icdd.com))*

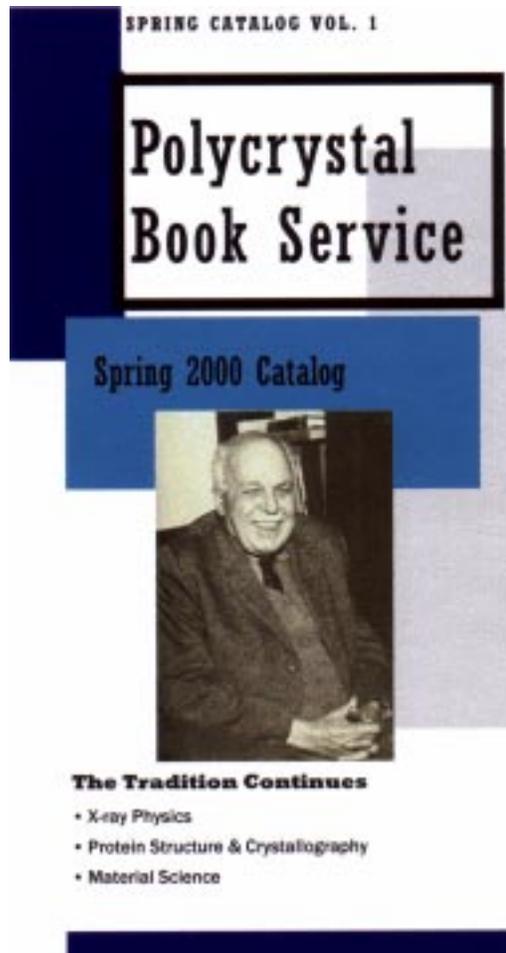
### Polycrystal Book Service Lives!!

Mert and Wade Adams are delighted to announce the transfer of operation of Polycrystal to Dan Carter and New Century Pharmaceuticals, Inc. in Huntsville, Alabama. We're pleased that Polycrystal will continue its long tradition of serving crystallographers world-wide and will be entering a new era with modern capabilities. We have had a wonderful 14 years of association with the ACA, IUCr, Denver X-ray Conference, and many dedicated customers. We'll see many of you at the ACA Banquet in July, and look forward to seeing many others as we continue to travel Wade's scientific meeting circuit. We strongly encourage you to continue to allow Polycrystal to be a book service to you in its new "5<sup>th</sup> Edition"!

*Mert and Wade Adams*

New Century Pharmaceuticals, Inc. (NCP) is very pleased to continue with the proud tradition of the POLYCRYSTAL BOOK SERVICE and can only aspire to the legacy and honorable stewardship of Wade and Mert Adams. Future plans for the PCBS are still in review, but will most certainly include an interactive website. The new websites for Polycrystal are under construction: [www.polycrystalbookservice.com](http://www.polycrystalbookservice.com) or [www.policbs.com](http://www.policbs.com). In the meantime orders may be placed by calling (256) 461-0024.

*Dan Carter*



### ***Press Release - Protein Solutions, Inc.***

ACA Corporate Member Protein Solutions Inc. (Charlottesville, VA) has announced a new light scattering instrument. The Dyna-Pro-MS/X Dynamic Light Scattering Instrument is capable of characterizing molecules in solution over a dynamic range from 1 nanometer to 1 micron. It represents a 500% increase in size range over its predecessor the Dyna-Pro-MS. The instrument can analyze the size, distribution, and hydrodynamic properties of biomolecules in solution within minutes. It was developed in response to a need for characterization tools that cover a broad range of applications including vaccine and drug delivery development, structure analysis, and basic characterization of molecules such as viruses, liposomes, monoclonal antibodies, nanoparticles, micelles, proteins, and peptides.

### ***ACA Thanks Exhibitors and Contributors to ACA 2000 in St Paul Minnesota***

***EXHIBITORS*** American Chemical Society; Area Detector Systems, Corp; Bede Scientific, Inc.; Beevers Miniature Models; Blake Industries, Inc; Bruker AXS, Inc; CCP4; Cambridge Crystallographic Data Centre; Compaq Computer Corp.; Cryo Industries of America; Emerald Biostructures, Inc; Gilson, Inc.; Hampton Research; International Union of Crystallography; Kratos Analytical, Inc; MAR USA, Inc; Molecular Simulations, Inc.; Molecular Structure Corp; NASA; Nonius Company; Oceaneering Space Systems, Inc.; Osmic, Inc; Oxford Cryosystems; Oxford Instruments; Protein Data Bank; Protein Solutions, Inc; Charles Supper Company; Wyatt Technology, Corp.

***CONTRIBUTORS*** Abbot Laboratories; Agouron Pharmaceuticals, Inc; BioCryst Pharmaceuticals, Inc; Bruker AXS, Inc; Cambridge Crystallographic Data Centre; DuPont Pharmaceuticals Company; Hampton Research; Hoffmann-La Roche Inc; International Union of Crystallography; Merck and Company, Inc.; Molecular Structure Corp; NASA; Nonius Company; Pharmacia & Upjohn; Silicon Graphics, Inc.; SmithKline Beechem; Charles Supper, Co.

### ***ACA Meeting Site Trivia***

***Only 1 state has been the site of 8 ACA meetings. Two others have hosted 5 meetings and two states have hosted 3 meetings. Two cities can claim both an ACA meeting and an IUCR Congress but only one site has the distinction of hosting both the 1st IUCR Congress and an ACA meeting. However, at least 4 sites have been the home to two ACA meetings and one city has hosted 3 ACA meetings. At least one site hosted at least two meetings but not in the same zipcode. Do you know where all these sites are? The answers are on the Cover (and scattered around in the pages of the Newsletter).***

**Charles W. Carter**  
(Vice President)



Professor of Biochemistry and Biophysics, School of Medicine, University of North Carolina, Chapel Hill, NC 27599-7260.

**Education:** B.A., Molecular Biophysics, Yale University (1967); M.S., Chemistry University of California at San Diego (1968); Ph.D., Biology / Chemistry University of California at San Diego (1972), Mentors: Joseph Kraut, UCSD (Ph.D); Aaron Klug, Medical Research Council Laboratory of Molecular Biology, Cambridge, UK (Postdoctoral, 1974).

**Professional activities:** U.S. National Committee for Crystallography, 1996-1998; 2000-2002; Chair, Program Committee Annual ACA meeting in Atlanta (1993); Co-chair with Gérard Bricogne, ACA *Transactions Symposium* "Solving structures using the Bayesian paradigm", 1993, Editor volume 1 of *METHODS: A Companion to Methods in Enzymology* (macromolecular crystal growth); co-editor with Bob Sweet of Volumes 276 and 277 of *Methods in Enzymology* (on macromolecular crystallography); review panels for the American Cancer Society (since 1988), and NSF (since 1997), NASA (1992), and NIH (ad-hoc and site visits). Co-Chair Gordon Conference on Diffraction Methods in Molecular Biology, 1996; Lecturer, FEBS short course in Macromolecular Crystallography, Aarhus, 1991; Lecturer, FEBS short course in Macromolecular Crystal Growth, Hamburg, 1998; Lecturer, EMBO Practical course in Crystallogenesi s of Biological Macromolecules, Strasbourg, 2000. Microgravity Research Subcommittee of the NRC Space Studies Board, 1998-2000; University Space Research Agency advisory committee, 1997-present.

**Research interests:** three redox-state behavior of tetranuclear iron-sulfur clusters in electron transport proteins; thermodynamic complementarity of polypeptide double helices and double-

stranded RNA; incomplete factorial sampling of multivariate experimental spaces and quantitative applications to problems in crystal growth screening, response surface optimization, and more recently, analysis of patterned combinatorial libraries; application of conditional probability methods developed by Gérard Bricogne, particularly phase permutation and likelihood scoring, to the solution of difficult macromolecular structures; determination of multiple crystal structures of *E. coli* cytidine deaminase and *B. stearotherophilus* *tryptophanyl-tRNA synthetase*, with application to questions of mechanistic enzymology and homology modeling.

**Statement:** I am honored to stand for election as Vice-President of the American Crystallographic Association. The ACA has been a wonderfully supportive professional home for me for many years, fostering both professional and personal growth, and I welcome the prospect of repaying that debt.

I cherish the study of the structure of matter in the broadest sense, and would hope to enhance the effectiveness of our entire constituency. The ACA is the natural home for all such research. It comprises an auspicious group of individuals sympathetic to preserving the considerable strengths throughout our profession. We are now witnessing unprecedented cross-fertilization across previously perceived boundaries. Small molecule Direct Methods have been strengthened and are now contributing significantly to macromolecular phase determinations. Bayesian statistical methods motivated by problems in macromolecular crystallography are contributing substantially to the study of powders, fibre diffraction, data processing at synchrotron sources, and to accurate electron density studies. These and other examples originated in good measure from the foresight of ACA leadership who have fostered inclusive courses and workshops throughout its history. I would work hard to extend these precedents, through effective liaisons between the ACA and other professional organizations, including member societies within the American Physical Society, the IUCr, and the Biophysical Society.

The coming decade will likely witness explosive growth of macromolecular structures, arising from intensive commitments to structural genomics on the one hand, and of new materials on the other hand. A variety of enabling tools will be developed and others will be strengthened. I would pursue vigorously the substantive issues arising from such growth. Some of these have concerned me as a member of the USNCCR: how to sustain the high quality of macromolecular crystal structures in the face of high-throughput technologies, how to manage and exploit existing and novel databases, and to protect intellectual property rights. These questions will pose new and perhaps unexpected challenges. I look forward to responding to them through responsive listening and effective actions.

A leadership role in preserving and extending all of these activities presents a challenge I would embrace joyfully.

**Jim Kaduk** (Vice-President)



Associate Research Scientist, Analytical Technology, BP Amoco p.l.c. Naperville Complex, P.O. Box 3011 MC F-9, Naperville IL 60566

**Education:** B.S. in Chemistry, University of Notre Dame, 1973; Ph.D. in Inorganic Chemistry, Northwestern, 1977.

**Professional Activities:** Secretary-Treasurer, U.S. National Committee for Crystallography (1998- 2000); ACA : representative to the AAAS Subsection on Industrial Science & Technology (2000-2002), Materials Science Special Interest Group Chair (1998), Apparatus and Standards Committee member (1994-1996), Service Crystallography SIG Chair (1990); International Union of Crystallography: member of the Subcommittee on the Union Calendar (1994-2002); Chairman of the Technical Committee and Member of the Board of Directors of the International Centre for Diffraction Data (2000-2002); Member of the Executive Committee of the Materials Research Collaborative Access Team (MRCAT) at the Advanced Photon Source; Visiting Lecturer, North Central College, Naperville IL.

**Research Interests:** I am driven by a profound desire to know “where the atoms are”. My current work spans a very wide range, including catalysts (zeolites, metal oxides, and supported metals), inorganic solids (superconducting, optical, and magnetic materials, as well as corrosion deposits), organic small molecules, coordination complexes (especially salts of aromatic carboxylic acids), synthetic polymers, and computational chemistry. Most of my current work involves what I like to call powder crystallography - answering structural questions using powder diffraction data (most industrial materials are not single crystals!) - and I am actively involved in solving structures *ab initio* from powder data. I still practice traditional single crystal crystallography, and it turns out that powder diffraction of biological macromolecules is not as hare-brained as it sounds!

**Statement:** Although it probably sounds trite to say it, it really is an honor to be nominated for ACA Vice-President. When people ask what I do for a living, I tell them that I'm a crystallographer. The typical reaction to that statement is a blank stare. My recent professorial experience has been teaching physical science to non-science majors (mostly elementary education majors). These experiences demonstrate to me just how far we have to go to achieve general science literacy, and appreciation of crystallography in particular. We need to share with the public the joy we get out of our science. The ACA can't do this task by itself; we need to work with others - perhaps AAAS, the Department of Education, museums, NIH, the press, and any other organization to get our message out. Crystallography is so fundamental that it gets lost in the “buzz” about the latest trends.

The growing trend toward laboratory certifications means that there is a need to develop standard procedures, methods which could be referenced. We might consider drafting “ACA approved” procedures to be used as the basis for analytical testing. As an organization, we need to ensure that members' skills are up to the demands of their jobs; I would like to see the ACA increase its involvement in continuing education. With the current dearth of formal crystallographic education

in the U.S., we might consider developing the standards which an “ACA certified” science department must meet.

The ACA is an efficient and well-run society. It sounds obvious, but one of Council's main jobs is to ensure that it continues to be well-run, and make sure that the headquarters staff have the tools that they need. I view the ACA as “owned” by its members (stockholders). To serve the members better, we need to understand them and their needs better. Perhaps we can apply “data mining” tools to develop a better picture of the ACA membership.

The American Crystallographic Association is a Regional Affiliate of IUCr. The name does not say “North American”. I would like to reach out to our Latin American colleagues, and see if it desirable for ACA to facilitate their interaction with the worldwide crystallographic community.

In the overall picture of science, the ACA is a small organization. We need to develop leverage, to maximize our influence. Our recent affiliation with AAAS represents a good step in this direction. We need to figure out how to use our affiliation to maximize the benefits to our members and our science. Crystallography is so fundamental to a variety of sciences that it is intrinsically multidisciplinary. We need to work with other societies to ensure that high-quality structural information is appreciated.

I have to admit that I fall into the materials science portion of the ACA, a collection of diverse interest groups which has become a smaller and smaller portion of the crystallographic universe. I'm an odd combination of a specialist and a generalist; I'd like to be able to cover all of structural science at a single meeting, but the world may be moving in a different direction. I consider ACA as my scientific “home”, and I'll try to attract materials scientists back to ACA meetings; but we may have to organize joint sessions on the applications of structural science to materials problems at other meetings - the Denver X-ray Conference, MRS meetings, and others. We need to maintain good relations with the newly-forming International Society for X-ray Analysis (IXAS). A challenge in all of this necessary

“outreach” will be maintaining our identity.

Crystallography is a database-intensive science. The ACA should encourage closer cooperation among the database organizations, and improved links between databases. It would be nice to use a common interface for multiple databases, and to be able to license them from a single place. As an organization, we need to pay attention to intellectual property issues, so that our access to data is not hampered. The ACA needs to be an advocate for the free exchange of scientific information, and an opponent of its commercialization.

Crystallographers have traditionally published their 3-(or higher)dimensional results in 2 dimensions, on paper. The Web makes visualization and access to crystallographic information possible in new ways, some which are still developing, and some we haven't thought of yet. The ACA (and IUCr) need to work with others to develop standards for the electronic publication of crystallographic information

Crystallography has changed from a small to a big science. The ACA needs to serve as an advocate of national user facilities (synchrotrons, neutron sources, and others) so that we have suitable access to the tools we need to do our science. Serving as such an advocate means treading a fine line between advocacy and lobbying.

While I can't promise to implement all these ideas, I present them to give you an idea of my vision for the future of ACA and crystallography. I look forward to serving the members of ACA.



**Douglas H. Ohlendorf**  
(Treasurer)

Professor of Biochemistry, Molecular Biology and Biophysics, University of Minnesota MN 55455

**Education:** A.B. & A.M. in Physics (1972) summa cum laude, Washington University. Ph.D. in Biochemistry (1978), Washington University

**Professional Activities:** Member ACA, AAAS, American Society of Microbiology, Biophysical Society, FASEB, Protein Society, Sigma Xi, Phi Beta Kappa. Coeditor, Journal of Applied Crystallography (1998-present). Secretary/Treasurer of Biomolecular SIG (1988-1990). Abstract Chair, Ninth International Conference on Biological Inorganic Chemistry (1999). Program chair 2000 ACA meeting. Fellow, Minnesota Supercomputing Institute (1996-present). Chair, Graduate Admission Committee, BBMB Graduate program (1998-present). Member, State Central Committee, Minnesota Democrat-Farm-Labor Party (1998-present).

**Research interests:** Structural foundation for biological function of macromolecules. Metalloenzymes. Virulence in gram positive pathogens.

**Statement:** The Treasurer of the ACA has 2 major roles. One is in handling the financial commitments of the organization and the second is as a member of the council. Regarding financial management, the ACA has become increasingly solid financially largely due to the conservative approach of the Council and the particularly the excellent current Treasurer, Jane Griffin. These resources need to be used to strengthen our annual conference. It can be difficult to get leaders in structural analysis to speak at our meetings because of the lack of funds for registration waivers let alone a travel subsidy. By focusing on keeping conference costs low and well-managed, we can allocate more money to the scientific program. This needs to be done while keeping dues and fees low.

As a member of Council I will be a strong advocate for education. Automation is becoming increasingly important not only in sample handling but also in diffraction data analysis. Also important is the analysis of our structures. Sessions on automation and on structural databases should be part of our conferences as well as sessions on new technologies. Crystallography is becoming more and more a tool to be used by technicians, often as a black box. The ACA has a responsibility to educate these newcomers into the science of the technique as well as the general community into the pitfalls that can occur. Our web site should have hyperlinks to sites to illustrate how crystallography works. In addition there needs to be regular sessions on education and training beyond the workshops.

**Edwin D. Stevens (Treasurer)**



Orleans, LA 70148.

Distinguished Professor of Chemistry, University of New Orleans, New Orleans, LA 70148.

**Education:** B.S.(Honors) Chemistry, Oregon State University (1969). Ph.D. Physical Chemistry, University of California, Davis (1973). Postdoctoral Fellow, State University of New York at Buffalo.

**Professional Activities:** Organized ACA Tutorial on Mathematical Tools in Crystallography (1980). ACA Apparatus and Standards Committee (1981-1983). Secretary/Treasurer ACA Small Molecule SIG (1983-1984). Co-Chairman of Gordon Conference on Electron Distributions and Chemical Bonding (1986). Member of IUCr Commission on Charge, Spin and Momentum Densities (1984-1993, Secretary 1987-1993). Secretary, ACS Louisiana Section (1985-1987). Chairman-Elect (1989) and Chairman (1990), ACA Small Molecule SIG. Vice-Chairman (1989) and Chairman (1990), Louisiana Section of the ACS. Local Co-Chairman, ACA National Meeting in New Orleans (1990). Candidate for ACA Vice-President (1991). Treasurer, Community

Church – UU, New Orleans (1986-1992) and Chair, Audit Committee (1993-1995).

**Research Interests:** Measurement of electron density distributions in small molecules and comparison with *ab initio* calculations.

**Statement:** As ACA Treasurer, my goal will be to continue the management of the financial affairs of the Association in a fiscally responsible manner, and to work with the ACA Council to minimize expenses while maintaining services to the membership.

**Patrick Van Roey (Continuing Education Committee - 3 year term)**



Research Scientist, Wadsworth Center, New York State Dept. of Health, Albany, NY 12201

**Education:** M.Sc. in Chemistry, University of Antwerp, Belgium (1976); Ph.D. in Chemistry, University of Calgary (1980); Postdoctoral Fellow, Medical Foundation of Buffalo (1980-1982).

**Professional activities:** Research Scientist, Medical Foundation of Buffalo (1982-1991); Associate Professor, Dept. of Biomedical Sciences, School of Public Health, SUNY/Albany (1994-1998); session organizer ACA 99; session co-organizer IUCr 99; member ACA, AAAS.

**Research interests:** Macromolecular crystallography with an emphasis of intermolecular interactions, including protein-carbohydrate and protein-DNA recognition and enzymology.

**Statement:** It has always been my opinion that the main purpose of the ACA's annual meeting is the education of the membership. This means making sure that graduate students and postdoctoral fellows get exposure to the fundamentals of the field, regardless of how automated the techniques become, while at the same time providing plenty of opportunity for everyone to keep up with the new developments.

**Winnie Wong-Ng (Continuing Education Committee - 3 year term)**



Research Chemist, Ceramics Division, National Institute of Standards and Technology (NIST), Gaithersburg, MD

20899

**Education:** B.S. in Chemistry (1969), Chinese University of Hong Kong; Ph.D. in Inorganic Chemistry (1974), Louisiana State University.

**Professional Activities:** Local co-chair of the 1998 Arlington ACA annual meeting; member of the US National Committee of Crystallography; chair of the Ceramics Subcommittee of the International Centre for Diffraction (ICDD, 1992-2000); chair of the ICDD Membership Committee (2000-present), chair of the Membership Committee of the Electronic Division of the American Ceramics Society (ACerS, 1998-present); member of ACA, ACerS, Sigma-Xi, Materials Research Society (MRS), and ICDD. Conferences organized: about 25 scientific symposia/sessions/workshops organized at the annual meetings of ACA, MRS, ACerS, and Denver X-ray Conferences. Author and co-author of more than 180 scientific publications.

**Research Interests:** Crystallography, crystal chemistry and phase equilibria of high temperature electronic materials. e.g. high Tc superconductors, microwave materials and ferroelectric materials, using single crystal, powder x-ray diffraction and neutron diffraction techniques; computer modelling of material properties using molecular orbital calculations; high pressure x-ray diffraction; and standard reference materials and data.

**Statement:** Continuing education is the key to progress in every scientific discipline. In recent years we have seen extraordinary developments in several scientific areas which have direct impact on the field of crystallography. First, new opportunities for crystallographic research in the area of materials science are available due to the continual discovery of new classes of technologically important materials. Many of these new materials

present immense crystallographic challenges due to their unusually complex structures. Secondly, rapid technical advancement in x-ray (and synchrotron x-ray), neutron, and electron diffraction of both single crystals and powdered materials has provided us powerful tools with which to unravel crystallographic problems. Also, various new methods of solving structures are emerging for both small and large systems. Third, computer technology has revolutionized our scientific activities, through the increased power of crystallographic databases, computer modeling, and the use of the World-Wide Web. At present we have the capability to make use of the crystallographic databases as a daily research tool for all areas of crystallography, ranging from small-molecule studies to protein crystallography. Performing modeling studies to understand structure-property relationships, formally limited by computer capability, has been made viable nowadays. The World-Wide-Web provides us with enormous opportunities to access various scientific information instantaneously, giving another powerful complementary tool for crystallographic science.

I propose a series of short courses or workshops to cover a wide spectrum of topics in various disciplines applicable to small and macromolecular crystallography. Possible topics include crystallography and modeling; advances in diffraction technology (neutron, electron, synchrotron, and conventional x-ray) and structure solution techniques; crystallographic databases as a research tool; non-ambient crystallography; and crystallography and phase equilibria.

I am honored to be considered as a candidate for membership on the Continuing Education Committee. If elected, I will work my utmost with other committee members to execute the mission of this committee. We will strive to bring knowledge of the latest advances in crystallography and related disciplines to the members of our Association.

**Philip Fanwick (Continuing Education Committee - 4 year term)**



Chemical Crystallographer, Dept. of Chemistry, Purdue University, W. Lafayette, In

**Education:** BS Tulane (69), MS (72), PhD(77) Iowa State, Post Doc Texas A&M

(77-79)

**Professional Activities:** Chair Service Sig (98), Organized ACA Symposium "Teaching Crystallography to Non-Crystallographers"(99)

**Research Interests:** Structure Solution, Crystallographic Programming, and Education.

**Statement:** The rapid changes in instrumentation and software have greatly increased the importance of crystallographic education. I have three main areas of concern. First, while the ACA workshops have done an excellent job of providing training, the information they provide needs improved dissemination and a longer lifetime. This could be accomplished using the web or CDs to supply the presentations by speakers, printed materials and any special software used. Secondly, there is an urgent need to train the next generation of crystallographers. It is important that the ACA provide materials and standards to ensure these crystallographers have a deeper understanding of the science than just how to solve structures. Third, crystallographic education for non-crystallographers is generally terrible. The ACA needs to coordinate with other scientific organizations like the ACS to ensure that both undergraduate and graduate students get an appropriate introduction to the technique and that what is taught is correct. A series of articles in J. Chem. Ed. could be helpful in beginning a dialog.

**Margaret E. Kastner**  
*(Continuing Education  
 Committee - 4 year term)*



Professor, Dept.  
 of Chemistry,  
 Bucknell  
 University,  
 Lewisburg PA  
 17837

**Education:** BS in Education (1972) Indiana University at South Bend, Ph.D. (1979) in Chemistry, University of Notre Dame

**Professional Activities:** Chair of the Susquehanna Valley Section of the American Chemical Society (1993), General Chair of the 13th Biennial Conference on Chemical Education (1994), Member of the US National Committee for Crystallography (1994-96)

**Research Interests:** Structure of transition metal complexes and development of crystallographic courseware.

**Statement:** The primary concern of the Continuing Education Committee has rightly been the enrichment and development of the membership itself. My primary concern in "continuing education" is thus atypical. As I age and watch the retirement and passing of so many of those who have brought crystallography to its current stage of development, I worry about the status of the "continuing" of crystallographic "education". As the teaching of crystallography moves from the formal full courses taught by traditional faculty members to less formal short-courses or hands-on training sessions taught by instrument vendors or staff crystallographers there will be a change in the knowledge base of the next generation of crystallographers. The clock will never turn back and models of teaching that were successful in the past will not be available in the future. How do we respond to the new realities?

**Candidates for ACA offices in 2001**

The Nominating Committee has selected the following candidates for the 2000 elections for ACA offices in 2001.

**Vice-President:** Charles W. Carter and James A. Kaduk  
**Treasurer:** Douglas H. Ohlendorf and Edwin D. Stevens

**Committees:**

**Continuing Education :**

**3 year term** Patrick Van Roey and Winnie Wong-Ng  
    **4 year term:** Philip Fanwick and Margaret Kastner

**Communications Committee :**

**3 year term:** Jung-Ja P. Kim and John S. Sack  
    **4 year term:** Jeanette Krause-Bauer and David Rose

To nominate write-in candidates for any of these offices write to the ACA Secretary: Lee Brammer Dept. of Chemistry, University of Missouri-St. Louis, 8001 Natural Bridge Road, St. Louis, MO 63121-4499, FAX (314) 516-5342, [lee.brammer@umsl.edu](mailto:lee.brammer@umsl.edu). Letters must be received by September 15, 2000 and must be signed by 5 supporting ACA members and include a signed statement by the candidate describing his or her qualifications. Statements from all candidates will be included with the ballots which will be sent to all members in October 2000.

**2000 Nominating Committee**  
**David Smith (Chair), Penelope Coddling and Alan Pinkerton**

**Jung-Ja P. Kim**  
*(Communications Committee  
 - 3 year term)*



Professor,  
 Department of  
 Biochemistry,  
 Medical College of  
 Wisconsin,  
 Milwaukee, WI  
 53226.

**Education:** BS in Chemistry, Seoul National University, Seoul, Korea; Ph. D. in Physical Chemistry, Cornell University. Postdoc at McMaster University and MIT

**Professional Activities:** Member ACA, ACS, ASBMB; Secretary/Treasurer (1995-1997) of BIOMAC SIG of ACA; member NIH BCB study section (1991-1995).

**Research Interests:** Structural studies on biologically interesting molecules, focusing on flavoproteins and mannose-6-phosphate receptors.

**Statement:** The world is evolving constantly, and ACA is no exception. ACA needs to be an active participant in this age of fast multimedia communication. Therefore, the newly evolved communications committee has a broader mission than its predecessor, the publications committee. It is an honor and privilege to be nominated for this committee. I will work hard to insure that the committee fulfills its mission.

**John S. Sack (Communications  
 Committee - 3 year  
 term)**



Principal Scientist,  
 Department of  
 Macromolecular  
 Crystallography, Bristol-

Myers Squibb Pharmaceutical Research Institute, Princeton, NJ.

**Education:** B.S. in Physics, Carnegie-Mellon Univ, (1975); Ph.D. Biophysics, Johns Hopkins Univ., (1981); Postdoctoral

Fellow, Univ. Alabama in Birmingham, (1981-1984); Post-doctoral Fellow, Rice Univ., (1984-1986).

**Professional Activities:** ACA Biological Macromolecules SIG (00), Member: AAAS, ACA, Protein Society.

**Research Interests:** Structure-based drug design; Macromolecular structure and function; Synchrotron Radiation.

**Statement:** I see the Communications Committee as having two major roles. One is to advise and monitor our current publishing activities and to consider possible new directions, in both print and electronic media, for the ACA. The committee also needs to be a voice for our community in evaluating and reviewing the editorial policies for X-ray crystallographic studies in major journals, and seeing if those policies are in the best interest of our membership.

The change in structure of the Communications Committee in 2001, with a larger membership and longer terms, should give us the resources and continuity needed to be a strong voice for the crystallographic community.

**Jeanette Krause Bauer**  
(Communications Committee - 4 year term)



Research Associate, Department of Chemistry, University of Cincinnati, Cincinnati, OH. Director, Crystallographic Facility (1991-present).

**Education:** B.S. Chem., Chemistry and Cellular-Molecular Biology, University of Michigan (1982); M.S., Inorganic Chemistry, Ohio State University (1987); Ph.D., Inorganic Chemistry, Ohio State University (1989); Postdoctoral Fellow, SmithKline Beecham Pharmaceuticals (1989-1991).

**Professional Activities:** Program Chair, ACA2003; Program Committee Member, 32nd Central Regional ACS Meeting (2000); Member of the Continuing Education (1997-1999) and Publications (1995-1997) Standing Committees; Member of the Program Committee &/or Session Organizer for the ACA annual

meeting (1993-1999); US Co-editor, World Directory of Crystallographers, 10th edition (1996); Chair (1997) and Secretary (1994-1995) of the Small Molecule SIG; Secretary (1995-1996) of the Service Crystallography SIG; Microsymposium Co-organizer, Seattle IUCr Congress (CGA-17) (1996); Program Committee Member, 24th Central Regional ACS Meeting (1992). Member of ACA, ACS, Pittsburgh Diffraction Society, AAAS, Protein Society, American Peptide Society.

**Research Interests:** Small molecule crystallography, methods of crystal growth, structure-activity relationships of biologically important small molecules and crystal engineering. Future research interests: Macromolecular crystallography.

**Statement:** The year 2001 marks a change in the way the ACA standing committees will be organized. The Publications Standing Committee becomes the Communications Committee and with the change comes new responsibilities. The high quality that the ACA has become accustomed to will remain forefront in the committee's involvement in the Newsletter and in other areas promoting the ACA.

The members of the ACA have been a valuable source of learning and inspiration to me as a crystallographer. I am pleased to accept the nomination and volunteer my services to the ACA. If elected I will strive to do my best to fulfill the duties of this committee.

**David Rose (Communications Committee - 4 year term)**



Professor, Department of Medical Biophysics, University of Toronto / Senior Scientist, Ontario Cancer Institute, 610 University Avenue, Toronto, Ontario M5G 2M9

**Education:** B.A in Biophysics. University of Pennsylvania, 1977; D.Phil in Molecular Biophysics, University of Oxford, 1981; Postdoctoral Associate, MIT, 1981-1984; Research Associate / Research Officer, National Research Council of Canada, Ottawa, 1984-1991.

**Professional Activities:** ACA member since 1986.

**Research Interests:** Crystallographic analysis of glycosyl hydrolase catalytic mechanism and development of inhibitors. Structure/function of ABC transporters. Antigen-antibody interactions.

**Statement:** Effective communication among scientists, between scientists and the general public and politicians, and between scientists and the business community is as important as ever. Our existence depends on an educated public that is convinced of the benefits of research to society's health and welfare. Organizations such as the ACA play a key role in this education process.

In the area of dissemination of scientific progress, electronic publication has established itself and will become the norm very soon. Key issues relevant to macromolecular crystallographers in particular, include the mechanism for reporting new structures. As the rate of new structures increases, especially with the accessibility of whole genome information and high throughput technology, the novel information content of most individual structures decreases. There is a need for discussion and implementation of new ways of measuring productivity, to supplement conventional publication. These might include validated depositions into the Protein Data Bank as one indicator, perhaps accompanied by short descriptive reports, since presentation in detail in mainstream journals will not be possible for many new structures. Even though their individual impact might be minimal, such structures should still be archived and acknowledged, much as crystallization reports are currently. Again, the ACA's role will be crucial in setting standards and gaining acceptance for new initiatives in the scientific research and funding communities.

*The ACA has met 8 times in Pennsylvania, 5 times each in California and New York and 3 times each in Massachusetts and Texas*

*ISAS Workshop at UGA, April 6-7, 2000*



Some thirty participants came to the UGA campus on April 6 & 7 for a workshop devoted to phasing of single wavelength anomalous

scattering (SAS) data using the ISAS program developed by Bi-Cheng Wang. The major aim of the technique is to phase protein data from single wave-length data using anomalous scattering differences. Proteins containing atoms with large  $\Delta f'$  are most likely to be successful. The most challenging application of ISAS is to phase data based on the sulfur anomalous scattering signal ( $\Delta f' 0.56$  at  $1.54 \text{ \AA}$ ). Since most proteins contain sulfur, this method, if generally applicable, could provide a fast and efficient way to determine protein structures. Already, in our hands, three proteins have been phased with only the anomalous signal from sulfur using synchrotron data measured with  $\sim 1.7 \text{ \AA}$  X-rays.

The first day of the workshop began with a discussion of the ISAS theory by B.-C. Wang and was followed by a discussion of the practical problems involved in application of the method by Zhi-Jie Liu and Chung-Jung Chen. The afternoon session provided hands-on practice with the ISAS program using already solved structures. The second day began with a discussion of the results from the first day. The next presentation by John Rose described the application of iron SAS data measured in house used in the structure determination of human ferrochelatase. Herbert Hauptman also gave a presentation about new ideas for direct phasing of macromolecules.



*A busy group working in the Molecular Graphics Lab*

A true UNIX version of the original ISIR/ISAS program suite with a simple user interface is being prepared by Zhi-Jie Liu and will be available for general distribution shortly. If you are interested in a copy of this program, please contact B.-C. Wang (wang@BCL1.bmb.uga.edu). Another ISAS workshop at UGA is planned for the near future.

Gary Newton

*Contributors to this Issue*

Cele Abad-Zapatero, Sidney Abrahams, Mert and Wade Adams, Helen Berman, Lee Brammer, Charlie Bugg, Robinson Burbank, Brian Burkhart, Bill Busing, Sue Byram, Charlie Carter, Dan Carter, Connie Chidester, Patti Coley, Bryan Craven, Louis Delbaere, Bill Duax, Fred Dyda, Marcia Evans, Philip Fanwick, Bert Frenz, Suzanne Fortier, Jenny Glusker, Dick Harlow, Michael Hart, Jim Kaduk, Isabella Karle, Jerome Karle, Charlys Lucht Kasper, Margaret Kastner, Jung-Ja Kim, Jeanette Krause-Bauer, Sally Lunge, Helen McDonnell, Gary Newton, Doug Ohlendorf, Joe Reibenspies, Tom Reiker, David Rose, Rueben Rudman, John Sack, David Sayre, Nathan Spielberg, Hugo Steinfink, Ed Stevens, Susan Strasser, Lee Supper, Patrick Van Roey, Winnie Wong-Ng, Elizabeth Wood, Christine Zardecki

Photos: Sidney Abrahams, Helen Berman, Sue Byram, Bill Duax, Judy Flippen-Anderson, Reuben Rudman, Hugo Steinfink.

*Letter to the Editor*

Just an observation re: the story from Lawrence Livermore National Laboratory and on the Newsletter cover (Spring 2000). The world's largest single crystals, often observed on cruises (but not by me yet, unfortunately) are frozen sea ice. In textbooks there are pictures of same taken through polaroids which give contrast between the individual grains which are on a much larger scale than this 'little' ADP crystal.

Michael Hart

*Key to Cover*

*Yellow = IUCr Meeting site*

*Red = ACA Meeting site*

*White = Future ACA Meeting site*

### 10th APS Users Meeting, Argonne National Laboratory, May 2-4, 2000

More than 500 people attended the Tenth Users Meeting for the Advanced Photon Source (APS), which was held on May 2-4, 2000, just a few days before the tenth anniversary of the 1990 ground-breaking for this world-class synchrotron source. The meeting, held in the APS Conference Center at Argonne National Laboratory near Chicago, consisted of two general sessions with invited talks on user science; a poster session and competition; six workshops; and several social events, including a banquet and sky show at Chicago's Adler Planetarium.

Of most interest to crystallographers were several talks in the first general session, one talk in the "Introduction to the APS" workshop, and a workshop entitled "Biological Studies for the 21<sup>st</sup> Century" organized by Janet Smith (Purdue University) and Jack Johnson (The Scripps Research Institute).

The **biological studies workshop** highlighted a wide variety of synchrotron radiation techniques and applications in structural studies with biological samples of increasing size and complexity. The presentations covered solution and single-crystal studies of viruses, medium- to high-resolution studies of other large macromolecular aggregates and complexes, and a variety of examples and applications of multiwavelength studies. In addition, advances in high-throughput methodology such as robotics for crystal mounting, beamline automation, and structure determination were presented.

Hiro Tsuruta (Stanford Synchrotron Radiation Laboratory) described the biological applications of small angle x-ray diffraction (Bio-SAXD) on beamline 4-2 used to obtain information about conformational changes, protein-protein interactions, and low-resolution envelopes. Particularly impressive were the extremely low resolution (600 to 250 Å) diffraction data gathered for viruses. These data make possible the *ab initio* phasing of virus particles by using an initial spherical model—a dream that some in the virus community had in the mid seventies. In addition, these low-resolution data allow a better calibration of electron microscopy data resulting in better initial phasing models. Tsuruta also discussed his stop-flow experimental setup to study the kinetic properties of biological systems away from the constraints of a crystal lattice. In particular, the systematic study of variables affecting protein folding are especially relevant.

Bill Wikoff from the Scripps Research Institute presented the methodology used to obtain the structure of two forms of the capsid of HK97, a double-stranded DNA bacteriophage. The capsid is the first T=7 structure that has been elucidated. The structure determination used the superb very-low-angle diffraction data (beginning at 200Å) obtained at Tsuruta's beamline. These data were used to radially scale the electron microscopy data (a critical step). The final and highest resolution data (5-3.5 Å) were collected at the APS (Beamline 14-BM-C). A staggering number of reflections (21 x 10<sup>6</sup>) were measured and reduced to a set of 4.8 x 10<sup>6</sup> unique reflections. The protein shell turned out

to be extremely thin (only 18 Å of a total 659 Å diameter) and presented an interchain crosslinking between Asn356 and Lys169 that results in the extreme stability of the capsid. Results like these are providing more and more evidence that virus capsids are not just inert envelopes.

Karin Reinisch from Harvard University described the current state of knowledge on the structure of reovirus core particles, which synthesize, chemically modify, and export viral mRNA into the cytoplasm of the host cell. Once again the dimensions of the proteins she works with are stunning: 750 Å in diameter, multiple copies of five different polypeptides, which crystallize in a cubic F432 cell of 1255 Å cell edge. The capsid protein has to perform several critical functions in the infective virus; it serves as a polymerase, a phosphatase, and a guanylyl transferase, as well as performing two different types of methylation (N7 and 2O') using S-adenosyl-methionine (SAM or AdoMet) as a cofactor. Reinisch showed the location of the majority of the active sites on the protein shell and discussed the important role of the 'turret' of the protein capsid (Reinisch et al., *Nature* (2000), 404, 960-967).

As an alternative to standard multiple wavelength anomalous diffraction (MAD) experiments, which are not always possible, Luke Rice of Yale University presented information on the use of single anomalous diffraction (SAD) in combination with solvent flattening and other density modification techniques to obtain interpretable maps. The concept, of course, is not new, but the pressures on beamline time coupled with pressures for high-throughput may rejuvenate this approach.

An intriguing approach and a beautiful structure were presented by Andrew Sharff from Cambridge University. He indicated that failure of standard MAD methods prompted him to *purposely* oxidize his Se-Met crystals of TolC (the efflux pump of extraneous substances in gram-negative bacteria). The protein is a 428 residue (47 KDa) polypeptide chain, which forms a homotrimer in the native membrane. Sharff suggested that in many cases heterogeneity of the redox state of the different Se-Met residues in the target protein may obscure the anomalous signal enough to prevent successful phasing. He was able to get a clean 'white line' of Se-Met after a brief (10 sec) exposure to 0.1% v/v hydrogen peroxide. The resulting structure was a 142 Å long protein structure with a porin-like (all beta sheet) domain, probably embedded in the membrane, and a gun-barrel-like extension (all helical) that probably spans the periplasmic space of gram-negative bacteria.

Michael Soltis from Stanford presented his plans to automate the vast majority of the elements in his synchrotron beamline to facilitate its use, reduce errors, and increase throughput. He presented schematics of sample holders and other hardware for a crystal mounting robot. Judging from the momentum that this kind of activity is getting in the structural biology community, it seems inevitable that breakthroughs can be expected in the not-to-distant future. (*Note: A workshop on beamline automation, which was held on May 11-12 at the Stanford Synchrotron Radiation Laboratory, brought together many of the groups working on this problem.*) All this activity has resulted in (1)

determination of larger complexes at higher resolution, (2) development of high-throughput screening methods, (3) extremely rapid structure determinations (important for structural genomics), and (4) the collection of amazing data at ultrahigh resolution (for instance B-DNA at 0.68; currently on line SSRL 9-1 and eventually also 9-2). The combination of the Biological Information Center (BIC), Structure Determination Core (SDC), and Crystallomics Core (CC) to form the Joint Center for Structural Genomics (JCSG) that he outlined, could make possible the determination of 5,000 new protein structures in the next five years.

Robert Rambo from Yale University presented his work on unraveling the structural mechanisms of protein targeting. Proteins are targeted for secretion or insertion into the cell membrane by using a signal recognition particle (SRP), which is a ubiquitous ribonucleoprotein complex. The interaction between the signal sequence recognition protein, SRP54/Ffh, and the 4.5S RNA of the SRP is mediated by the universally conserved M-domain, with a pico-molar binding constant. An RNA fragment was engineered for optimum crystallization, and the protein-RNA complex was crystallized in a form that diffracts to 1.52 Å. Multiple wavelength anomalous diffraction (MAD) with Se-Met was used to phase the structure. The recognition is based on a helix-turn-helix motif, but it was not clear whether it corresponds to the 'canonical' helix-turn-helix motif characterized in the DNA-protein interactions. Of note is the fact that all of the amino acids within the M-domain and the nucleotides in the 4.5 SRNA that form the interface are universally conserved. The role of a number of well-ordered  $K^+$  and  $Mg^{++}$  ions, as well as water molecules in the interface, was briefly discussed.

To allow ample time for discussion, the organizers saved the most intriguing presentation for the end. Sean McSweeney (EMBL-Grenoble Outstation) reviewed the published work (Weik et al. *PNAS* (2000), 97, 623-628; Ravelli & McSweeney, *Structure* (2000), 8, 315-328; Burmeister, *Acta Cryst.* (2000) D56, 328-341) on damage to biological samples exposed to synchrotron radiation. The published work documents specific, time-dependent changes detected in protein structures exposed to radiation: disulfide bond breakage and decarboxylation of acidic residues are the best characterized. The results suggest the presence of 'strained' (in the terminology of the speaker) regions of the protein that are particularly affected. A lively discussion followed McSweeney's presentation. Many questions still remain unanswered, but this area of inquiry will continue to be of interest in view of the increasing use of well-focused undulator beamlines. The full ramifications of localized radiation damage in proteins are still unexplored.

The workshop entitled "**Introduction to the Advanced Photon Source**" organized by Dean Haeffner of the APS was designed to provide new and/or inexperienced users with a comprehensive overview of the radiation properties and potential applications of the APS. A series of talks highlighted work in various disciplines. Thomas Irving (Illinois Institute of Technology) enthusiastically described studies with non-crystalline biological materials, where the high flux and low angular divergence of undulator radiation

provides a "nearly ideal" probe to study small, weakly diffracting species and conduct dynamic studies of biological samples in solution.

The first general session on User Science began with a memorial talk given by Andrzej Joachimiak of Argonne National Laboratory as a tribute to Paul Sigler of Yale University, who passed away recently. Joachimiak began by reviewing the spectacular trajectory of Paul's work in structural biology. A physician by training, Dr. Sigler began his work in structural biology with chymotrypsin, followed by initiator tRNA and phospholipases. In 1981, Sigler began his 'adventure with transcription' by describing several trp repressors that unveiled allosteric regulation in transcription. In the same vein, he studied TBP/TATA complexes, glucocorticoid/DNA, RXR-TR/response element, NF-kB/IB site and others. He also extensively studied G-proteins and proteins associated with signal transduction: G-transducin, heterotrimeric G protein, visual arrestin, fosducin/G complex. Most recently, his studies on the structures of chaperonin proteins (GroEL, GroES and related complexes) were designed to elucidate the function hidden behind the magnificent structures that he and his colleagues presented to the community. Especially noteworthy was the interest and support Sigler demonstrated for synchrotron sources. He served as an early member of the APS Users Organization and as Chair of the Principal Users Group of the APS Structural Biology Center. Joachimiak entitled his tribute "A Tour de Force in Structural Biology." Those who knew Paul Sigler would agree that the title was fitting. The structural biology community is saddened by the untimely end to his career but continue to be inspired by his enthusiasm, zest for life, and scientific vision.

The presentation by Lois Pollack (Cornell University) discussed in detail the application of stop-flow techniques and extremely rapid fluid mixing methods to study protein folding. By using nanofabrication, the Cornell group has been able to produce mixing chambers that achieve uniform mixings on the submillisecond time scale. These chambers are used in small-angle x-ray scattering studies to analyze the effect of environmental parameters such as pH in protein folding. Other environmental variables (possibly temperature and denaturants) will be considered next. The future potential for these non-diffraction techniques is enormous.

Abstracts of all talks presented in the general sessions and workshops can be obtained on the meeting Web site: <http://www.aps.anl.gov/conferences/10um/>

*Cele Abad-Zapatero and Susan Strasser*

### *Bruker Area Detector Users Meeting - SADUG, Texas A & M, March 16-17, 2000*

SADUG 2000 was held at the Department of Chemistry, Texas A & M University on March 16 and 17. The invited speakers were Abraham Clearfield, Sue Byram, Roger Durst, George Sheldrick, Charles Campana, Victor Young, Peter Muller, Joseph Reibenspies, Roland Boese and Robert Sparks. The mornings sessions involved short seminars on varying subjects while the afternoon sessions were dedicated to hands-on with interactive programs on the two departmental SMART1000 CCD diffractometers and computer systems. Several subjects were covered in the two-day sessions. Professor A. Clearfield began the meeting as the keynote speaker. He discussed the state-of-the-art structure solution from x-ray powder diffraction data. We were intrigued to learn that 60 atom structures can now be solved and refined by the powder method and that we are well on our way to "routine" structural investigations with powder data. One



*Joe Reibenspies and Bob Sparks look over a pre-P1bar that came to Texas A&M over 30 years ago*

point Professor Clearfield stressed is that the cooperation of the single-crystal and powder communities will present new opportunities in structural elucidation. Other speakers presented sessions on the fast moving state of crystallographic hardware and software.

Sue Byram gave a short presentation on what is new at Bruker. Roger Durst brought us the latest information on the next generation of CCD based detectors and the new and expanded use of the monocapillary collimators. He also presented a demonstration on maintaining the SMART1000 CCD cameras. Charles Campana discussed the latest crystallographic software and how to use these programs for better data collection, structure solution and refinement. Charles also spent the afternoon sessions with users, who had brought their most difficult structures and crystals. George Sheldrick introduced his new improved version of SADABS at the user's meeting. The new version (now out in beta release) has many new features that have already proven useful in both absorption correction and inter-frame scaling. George was also available after his session to demonstrate SADABS many uses to an eager audience of users and to interact with individuals. Victor Young presented an excellent seminar on twinning, followed by working up a specimen on a SMART1000 CCD diffractometer. Users could see first hand the complications and the solution of a twinned crystal. Victor then spent the afternoon session helping individuals with twinned crystals and data that they had brought with them. Peter Muller demonstrated some unique crystal handling techniques on the diffractometer. Using a low temperature tabletop cooling device he was able to mount crystals we have lovingly named "instant death". For the first time we were able to collect data on crystals, mounted in a loop, without our normal crystal protectants (mineral oil and paratone). The crystals on the examination slide remained

intact under a stream of cold nitrogen. Peter returned again and again to the examination slide until he found a suitable crystal. Crystals that normally last only a few seconds at room temperature remained usable for several hours with the tabletop cooling device.



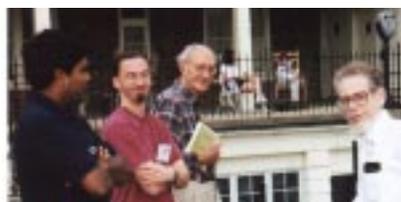
*Lee Daniels, Larry Dahl and Ken Hardcastle trading tips on doing structures*

Joseph Reibenspies demonstrated the collection of powder data on the SMART1000 CCD (Mo radiation). He also collected data on unknown samples provided by the users. Remarkably, X. Ouyang was able to index these powder patterns and provide qualitative analysis of their initial structures. Roland Boese suggested a new use for our older point detection diffractometer as an in situ crystal growth and data collection instrument. Employing lasers, Roland was able to grow crystals in capillaries on the single-crystal diffractometer and then collect the data. Robert Sparks introduced us to his latest software, titled FINDSYM. Bob's software is useful in determining symmetry and missed symmetry. Based upon known algorithms, FINDSYM incorporates additional guidelines and suggestions to the users in ways of selecting symmetry and transforming data. Bob spent the afternoon sessions interacting with and helping users with their crystallographic problems. At the users meeting a unique opportunity was realized when we seated a panel of world-renowned experts on twinning. The panel seated Charles Campana, George Sheldrick, Victor Young and Robert Sparks and was hosted by X. Ouyang. We discussed a wide variety of topics, such as whole molecule disorder and crystal twinning versus cracked crystals. The afternoon sessions proved to be a delightful mix of users in one-on-one situations with the "old" masters. Many computers and laptops sprang up on empty benches and individuals shared their experience and knowledge to solve and refine structures. Peter White, for instance, allowed us to search the CRYSMET database via his new interface program. Peter Muller, Charles Campana, Victor Young and many others mounted and collected data on some of the most difficult samples that this lab has seen. The afternoon broke down in a form of "controlled chaos" where the general interaction of users was the norm and various techniques were discussed and demonstrated for small to large groups of users. In the two days of "controlled chaos" no less than twenty structures were either solved or refined to some degree of completion. We ended the sessions as we had begun them with small informal groups passing their knowledge between themselves and everyone (including the old masters) learning something new.

*Joseph H. Reibenspies*

**The 28<sup>th</sup> Mid-Atlantic Protein Crystallography Workshop, Hilltop House, Harpers Ferry, WV, May 3-5, 2000**

The meeting was organized by David Davies, Fred Dyda, Jim Hurley and Wei Yang of the National Institute of Diabetes, and Digestive and Kidney Diseases. The 118 participants enjoyed the dramatic views of the Potomac valley from the terraces and the walks to the town rich in Civil War history. The weather could not have been more cooperative: a high pressure system prevailed throughout the meeting, offering plenty of sunshine and pleasantly warm temperatures. Financial support for the meeting was provided by twelve generous corporate sponsors. The organizers also acknowledged the substantial logistical help provided by Gary Gilliland of the National Institute of Standards and Technology and the University of Maryland.



*Bertram Canagarajah, Tim Umland, meeting organizer David Davies and Gerson Cohen*

The scientific program was kicked off Wednesday afternoon with the keynote address by Brian Matthews (University of Oregon) who gave an enlightening summary of the structural behavior of T4

lysozyme derived from the large number of mutant structures that his laboratory solved. Especially lively discussion was prompted by his observations regarding the relative temperature factor distributions of main chain and side chain atoms, and also by his new results about the contested issue of solvent molecules in hydrophobic pockets.

Cynthia Wolberger chaired the Wednesday evening session on protein-protein and protein-DNA complexes. Jeffrey Boyington (NIAID) described several complex structures of natural killer cell receptor peptides and their Class I MHC ligands. Galina Oblomova (NIDDK) spoke about the recent success of solving the structure of the Taq MutS DNA repair protein complexed with dsDNA containing a mismatch. This structure offers intriguing insights into the mechanism of mismatch repair. Jun Aishima (Johns Hopkins University) spoke about his structure of a MAT alpha2 homeodomain complexed with DNA. Surprisingly, the DNA contains a Hoogsteen base pair and furthermore the stoichiometry of the complex is different from the expected 2 protein molecules per one DNA; rather, these were found in a 4:1 ratio in the structure. This is the first time that Hoogsteen base pairing has been seen in undistorted DNA. Murray Junop (NIDDK) talked about his new results on the structure of the human XRCC4, a molecule involved in double strand break repair and in non-homologous DNA end-joining. The last talk of the evening was delivered by Di Xia (NCI) who spoke about how he used anomalous scattering of iron to look at redox induced conformational changes in the cytochrome bc I complex. After the session, participants occupied the various rooms and terraces of the Hilltop House for lively discussions.

On Thursday morning, Bob Kretsinger of the University of

Virginia chaired the methods session that spanned all areas from crystallization to the analysis of solved structures. Lance Stewart from Emerald Biosystems (also one of the meeting's corporate sponsors) spoke about their work on developing a new database-oriented software application to monitor and rationalize the outcomes of crystallization experiments in a highly organized and easily accessible fashion. One of the most original methodological results was described in Jane Ladner's (CARB, University of Maryland) presentation about the use of short crystal soaks in nearly saturating concentrations of salt solutions as a way to achieve cryoprotection. These results are probably very significant considering that the usual drawback of conventional methods of cryoprotection - the increase in mosaic spread - seems to be absent using this new method. Peter Sun (NIAID) spoke of his experiences using mass spectrometry to identify heavy atom derivatives, and Narmada Thanki (RCSB and NIST) spoke of efforts to establish uniformity in the structure data base to allow for more powerful searches. Finally, Jane Richardson (Duke University) spoke about her new and "ultimate" rotamer library that should make structure building easier and structure quality better. Users of the graphic program 'O' can already use this library, since it has been encoded as the appropriate 'O' data block

The next session, chaired by Osnat Herzberg (CARB and University of Maryland), featured the first results from structural genomics efforts and also some previously not seen protein folds. Highlights included Thomas Martin (University of Virginia) who introduced Met residues to facilitate phasing to solve his structure of a potential drug target in the mitomycin C resistance pathway. Christine Wright (University of Virginia) described the interesting and unexpected structure of GM2-activator protein that shows a large hole in its central part, presumably involved in lipid binding. Yosuke Tsujishita (NIDDK) described his structure of the STAR domain that is involved in lipid transport. Sandra Gabelli (Johns Hopkins University) described a Nudix hydrolase structure that exhibits a novel fold and also an interesting dimerization motif involving domain swapping. Closing the session was the interesting results of Artem Evdokimov (NCI-FCRDC) concerning the structure of YopM, a leucine-rich effector protein. Although its exact function is unknown at this point, the crystal packing seems to suggest tunnel formation, which may well be related to its biological function.

Sixteen posters were presented in the afternoon's poster session. The newly established Paul Sigler poster prize was given to the best of these as judged by a panel that this year consisted of David Davies and Brian Matthews. The memory of Paul Sigler is of course relevant to the Mid-Atlantic region, since it was in David Davies' laboratory at NIH in 1962 where Paul started his career in structural biology after he finished his medical degree. This year, the prize was awarded to Sean Johnson (Duke University) for his outstanding presentation on the mechanism of fidelity of DNA polymerase.



*Jane Richardson*



*Sean Johnson - Winner of the Paul Sigler Poster Prize*

The evening session on the topic of experimental phase determination by MAD and SAS was chaired by David Davies. Celia Cheng (CARB) described a rather difficult structure determination using 66 Se atoms in the asymmetric unit to solve a structure consisting of a total of 2160 amino acids. Initial attempts to locate the anomalous scatterers using direct methods alone as implemented in Shake and Bake failed; however, the combined Patterson and direct methods approach in the new (yet-unreleased) version of SHELX succeeded with the help of the authors of the program. The next two talks presented novel structures determined by the new halide ion MAD method (Br in both cases) developed by Zbigniew Dauter of the NCI. Jonathan Ho (NIDDK) solved the structure of the GAF domain that is involved in signaling processes using a NaBr soak while David Hoover (NCI-FCRDC) described a case involving the human beta defensin 2, where he initially gave up on the structure solution but later succeeded with the help of Zbigniew Dauter. The session was concluded by a presentation given by Zhi-Jie Liu (University of Georgia) who talked about some recent experiences using Single Wavelength Anomalous Scattering from a variety of scatterers as the sole means of experimental phase determination.

Honoring the tradition of the Mid-Atlantic meetings, Saturday morning was spent with informal and detailed workshop presentations. First, Thomas Schneider (University of Gottingen) spoke about the new SHELX program package with a particular focus on the ways and tricks for locating a large number of anomalously



*Jia Li, Zbigniew Dauter and meeting organizer Jim Hurley*

the program is still in the development stage, the authors encouraged everybody to send them their most difficult problems so they can work them out and also so that they can further optimize the package. Zbigniew Dauter (NCI) gave an very enlightening talk describing how he arrived to the realization that halide phasing might indeed be a real possibility, talked about his first successes, and gave much useful advice to new implementers of the method. Finally, Brian Chait (Rockefeller University) gave a much appreciated overview of using mass spectrometry to assist crystallization efforts and described his latest results on the application of mass spectrometry to obtaining substantial amounts of structural information on nuclear transporters.

A tentative decision was made to hold next year's meeting on the Charlottesville campus of the University of Virginia.

*Fred Dyda*

*58th Annual PDC Meeting, Pittsburgh, PA, October 26-28, 2000*

The Pittsburgh Diffraction Society will hold its 58th Annual Meeting from Oct 26-28, 2000 at the Holiday Inn Pittsburgh Airport. This years conference will have something for everyone with sessions on small angle scattering, powder x-ray diffraction, and macromolecular crystallography. So, with your participation, we expect many lively discussions on these wide ranging areas.

The program will begin Thursday Oct. 26 in the morning with a session on "Modern Methods of SAXS and SANS" and will be hosted by Hiro Tsuruta and Terrence Sabine. Topics will include recent advances in small angle scattering using both x-rays and neutrons and new methods being developed for these areas.

The Friday session, hosted by Bill David, is entitled "Powder X-Ray Diffraction Methods for Structure Solution and Refinement". Topics will include new methods for structure solution from powder x-ray diffraction and refinement techniques by Reitveld methods.

The Saturday session, for the macromolecular crystallography community, is entitled "Phasing Methods in Protein Crystallography". Hosted by Chang-Ill Ban and Wayne Schultz, topics of interest to those who like to phase their proteins include uses of SnB in solving large Se-Met problems and other new breakthroughs in getting around that pesky phase problem.

A poster session to be hosted by Charles Lake will be held Thursday evening during the mixer and will remain on display throughout the conference. The Chung Soo Yoo award (\$200) is made to the best student poster presented at the meeting. Student presenters must be present to meet the judges at the poster session on Thursday. Abstracts are due to Brian Burkhart (see below) before Sep. 15, 2000.

The Sidhu award will be presented for the best contribution to crystallography or diffraction by an investigator who obtained the PhD after October 1, 1995. A nomination package including cv and noteworthy reprints must be forwarded to Brian Burkhart (see below) by Sep. 29, 2000. The awardee will receive a prize of \$500 and will give a presentation at the symposium.

Accommodations are available at the conference hotel (1-800-HOLIDAY) for \$85/night. There are many other hotels in the area so more information will be provided in the meeting mailer. The meeting dinner will be held Friday night.

Further information about this meeting will be made available on the PDS web site at <http://www.pitt.edu/~geib/pds.html>. For more information on the conference and/or to submit abstracts or nominations please submit materials to:

Brian Burkhart Hauptman-Woodward Institute, 73 High Street, Buffalo, NY 14203 phone: 716/856-9600 FAX 716/852-6086 burkhart@hwi.buffalo.edu

*Brian Burkhart*

## Meeting Calendar

*In order to conserve space and paper, contact points for most meetings announced in previous newsletter issues will not be repeated. More complete information can be found in back issues of the newsletter.*

### JULY 2000

**22-27 ACA '00 St. Paul, MN.** Local Chairs: Bill Gleason (UMN) and Victor Young (UMN). Program Chair: Doug Ohlendorf (UMN).

**30 - Aug. 3 Teaching Crystallography to Undergraduate Symposium at 16<sup>th</sup> Biennial Conference on Chemical Education, Ann Arbor, MI.** Contact Prof. Guy Crundwell (crundwellg@ccsu.edu) or visit the BCCE website at <http://www.umich.edu/~bcce/>.

**31 - Aug. 4 Denver X-ray Conference, Denver, Colorado, USA.** See web page at <http://www.dxcicdd.com/>. Contact: Denise Flaherty, Conference Coordinator, ICDD, 12 Campus Blvd., Newtown Square, PA 19073-3273, Phone: 610-325-9814, Fax: 610-325-9823, E-mail: flaherty@icdd.com.

### AUGUST 2000

**19-23 8th International Conference on Intelligent Systems for Molecular Biology, San Diego, California USA.** See <http://ismb2000.sdsc.edu>

**25-31 19th European Crystallographic Meeting ECM 19, Nancy, France.** Chair: Claude Lecomte. e-mail: ecm19@lcm3b.u-nancy.fr. URL: [www.lcm3b.u-nancy.fr/ecm19/](http://www.lcm3b.u-nancy.fr/ecm19/).

### OCTOBER 2000

**11-15 10<sup>th</sup> International Symposium on Small Particles and Inorganic Clusters (ISSPIC), Atlanta, GA**

The Georgia Institute of Technology's School of Physics announces that it will be hosting the tenth annual International Symposium on Small Particles and Inorganic Clusters (ISSPIC). The five-day symposium will be devoted to a broad and balanced overview of new results, emerging trends and perspectives pertaining to the physics and chemistry of clusters. The symposium aims at providing an interdisciplinary forum for presentation and discussion of fundamental and methodological aspects of gas phase and supported clusters, nonoscale cluster-based materials, and nanometer scale systems through application and technologically oriented developments. Program fee is \$410 (\$270 for students). More information can be found at <http://www.physics.gatech.edu/isspic10/>

**26-28 Pittsburgh Diffraction Conference, Pittsburgh, PA.** Contacts: Bryan Craven, President. Chemistry Dept., IUP. 1491 Donahue Road, Creekside, PA 15732. (724)-397-9211. [alpacone@mail.microserve.net](mailto:alpacone@mail.microserve.net). Brian Burkhart, President-elect. HWI, 73 High St., Buffalo, NY 14203-1196. (716)-856-9600, ext 313. [burkhart@hwi.buffalo.edu](mailto:burkhart@hwi.buffalo.edu)

### SEPTEMBER 2000

**9-11 RSC Dalton Discussion 3 on Inorganic Crystal Engineering, Bologna.** See <http://www.rsc.org/lap/confs/daltondisc3.htm>

### JULY 2001

**21-26 ACA '01 Los Angeles, CA.** Local Chairs: Katherine Kantardjieff (CSU-Fullerton) and Dan Anderson (UCLA). Program Chair: Duncan McRee (Scripps).

**ACA Summer Course in Crystallography, Georgia Center for Continuing Education University of Georgia, Athens, GA,** <http://BCL15.bmb.uga.edu/aca2k.html>

### MAY 2002

**25-30 ACA '02 San Antonio, TX.** Local Chairs: Ray Davis (UT Austin) and Marv Hackert (UT Austin).

### AUGUST 2002

**6-15 19th IUCr General Assembly and Intl. Congress of Crystallography, Jerusalem, Israel.** Contact: J. Bernstein, Ben Gurion University, Beer Sheva, Israel.

## 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.

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

### Crystallography of Biopolymers - Full Professor

Universität Wien Formal - Und Naturwissenschaftliche Fakultät: In the context of the installation of a center for Molecular Structural Biology the University of Vienna invites applications for a full professorship in Crystallography of Biopolymers

The applicant should have research experience in the area of crystallography of protein and/or nucleic acids. He or she is expected to participate in the university teaching program of molecular structural biology. For additional information please visit the website [www.itc.univie.ac.at/](http://www.itc.univie.ac.at/)

Requirements for the appointment are a PhD or an equivalent degree from a university, documented achievements in research including publications in international scientific journals as well as experience in teaching at universities. The University of Vienna is an equal opportunity employer. With a view towards increasing the proportion of female professors, the University of Vienna specifically encourages female candidates to apply.

Applications including a curriculum vitae and a list of publications are to be submitted not later than September 15, 2000, to the Dean of the Formal- und Naturwissenschaftliche Fakultät, Prof. Dr. Marianne Popp, Universität Wien, Dr. Karl-Lueger 1, A-1010, Wien, Austria.

### Macromolecular Crystallographer:

Pharmacia has an opening for a Research Scientist in the Macromolecular Crystallography Group at Kalamazoo, Michigan. The scientist will conduct research on the structural biology of novel pharmaceutical targets to expand an existing structure-aided drug design effort. In collaboration with crystallographers, medicinal chemists and other program team members, the scientist will crystallize proteins, and solve and interpret structures to support drug discovery. The new scientist will join an established, well-equipped crystallography group.

The strong candidate will have a Ph.D. in Chemistry, Biochemistry or related field with extensive research laboratory experience and a strong record of success in crystallographic structure determination. Experience with molecular biology, protein chemistry, or crystallization that complements existing crystallography group expertise is highly desirable. The scientist will collaborate with a diverse assembly of protein chemists, molecular biologists and synthetic chemists on drug discovery program teams, and so must possess strong communication skills and command the respect of his/her peers. Apply as indicated in the next ad referring to position #900913

### Crystallization Biochemist, BS/MS:

The successful candidate will work as a member of the macromolecular crystallography laboratory. Responsibilities include the preparation of proteins and ligand complexes for crystallization experiments. This work requires the ability to set up and analyze a variety of macromolecular crystallization experiments with minimal supervision. M.S. or B.S. in Biochemistry. Experience in routine biochemical and biophysical techniques is required.

For confidential consideration apply on-line at [www.pharmacia.com](http://www.pharmacia.com) (hyperlink to Pharmacia and Upjohn, Employment Opportunities) or send your resume and a description of your research experience to: Dr. Eric T. Baldwin, Structural, Analytical and Medicinal Chemistry, 7255-209-102; Pharmacia; 301 Henrietta Street; Kalamazoo, MI, 49007, USA. E-mail: [eric.t.baldwin@am.pnu.com](mailto:eric.t.baldwin@am.pnu.com). Pharmacia is an equal opportunity employer, we value a diverse combination of ideas, perspectives and cultures. Refer to position #900087

### Francis Eppes Scholar in Macromolecular X-ray Crystallography

The structural Biology program of Florida State University is seeking a distinguished macromolecular X-ray crystallographer to fill an endowed chair position. The chair is named after Francis Eppes, a founder of the University and a nephew of Thomas Jefferson. The holder of this position will be a full professor in the Department of Biological Science.

The Structural Biology Program at FSU consists of eleven core

faculty -four in macromolecular X-ray crystallography, three in NMR, two in EPR spectroscopy, one in cryo-EM and one in mass spectroscopy. Searches are underway to fill two additional endowed chairs in high resolution NMR and bio-computational chemistry. In addition, significant faculty hires in computational structural biology are anticipated in association with FSU's new School of Computational Science and Information Technology. Structural Biology is strongly complemented by other multi-disciplinary research programs at FSU such as the National High Magnetic Field laboratory, Materials Sciences (MARTECH) and Biomedical Engineering.

A Search Committee has been established to identify candidates. The committee consists of Drs. Ross Ellington (Chair), Don Caspar, Michael Chapman, Betty Gaffney, Hong Li, Ken Roux, and Ken Taylor. Nominations or applications (with letter of application, curriculum vitae and list of three potential referees) should be sent to: Dr. W. Ross Ellington, Eppes Scholar Search Committee, Department of Biological Science, Florida State University, Tallahassee, FL 32306-4370

## Positions Previously Listed

### Postdoctoral Position

The Department of Molecular Biology and Biochemistry in the School of Biological Sciences at the University of California, Irvine, invites applications for a 100% time postdoctoral position in the area of macromolecular X-ray crystallography. Applicants must have experience in data collection, phasing, map interpretation and structure refinement. The areas of research would be structural immunology, viruses, and RNA structure. Send letter of application, curriculum vitae, and names of three references to Professor Alexander McPherson, MB&B Department, 560 Steinhaus Hall, UC-Irvine, Irvine, California 92697-3900 or email to: amcphers@uci.edu. The University is an equal opportunity employer.

### Diffraction Specialist

The Department of Chemistry and Biochemistry at Brigham Young University (BYU) invites applications for an X-ray Diffraction Specialist, a full-time tenure-track position. This faculty member will be expected to supervise the X-ray laboratory, to provide solid state X-ray structural data for small molecules and to teach graduate and undergraduate chemistry classes. Expertise in a range of structural methods is highly desirable. A Ph.D. in Chemistry is required. A letter of interest outlining experience and goals, a CV, publication list, and three letters of recommendation should be sent to the X-ray Specialist Search Committee, Dept. of Chemistry and Biochemistry, Brigham Young University, Provo, UT 84602-5700. Review of applications will begin on April 21, 2000 and continue until the position is filled. BYU is sponsored by the Church of Jesus Christ of Latter-Day Saints (LDS, Mormon), and is an equal employment opportunity employer. Strong preference is given to LDS applicants. Faculty are required to abide by standards consistent with LDS values.

### Postdoctoral Fellowships

Several postdoctoral fellowships are available in our laboratory to work on a number of medically relevant structural biology projects. The projects are all embedded in exciting structure-based drug design collaborative networks. Most of the projects are aimed to combat major infectious diseases, while one is also of major importance for cancer. A brief description of the projects is as follows:

1. Structural investigations of the biogenesis of unique organelles, called glycosomes, in Trypanosomatids which are protozoa responsible for several of the most important infectious diseases world wide. The glycosomal matrix proteins are all synthesized in the cytoplasm after which they are transported into the glycosome via a most unusual and interesting yet far from completely understood import mechanism. This process somehow involves almost two

dozen different proteins called "peroxins". Structure-based inhibitor design projects, aiming at discovering selective inhibitors of this import process, will be initiated immediately once crystal structures have been elucidated.

2. Structure-based drug design projects focusing on glycosomal proteins from *Trypanosoma brucei* and *Leishmania* species. These are crystallographic studies in close collaboration with medicinal chemists, molecular modelers and parasitologists. The aims are (i) to improve the affinity of very promising inhibitors already developed in the course of the project, and (ii) to discover and design entirely novel inhibitors of other target proteins.

3. Crystallographic investigations on human and malaria topoisomerase I. We not only wish to understand the mode of action of known topoisomerase inhibitors, but are also collaborating with synthetic chemists to develop novel inhibitors on the basis of our crystal structures, combined with molecular modeling and combinatorial chemistry approaches.

4. Structural studies on components of members of the very large pyruvate dehydrogenase multi-enzyme complex family. These are wonderful, multi-million Dalton complexes with a highly symmetric core surrounded by a very dynamic and flexible arrangement of dozens of additional proteins.

The positions require a great interest in medically oriented protein crystallography and excellent crystallographic skills. Experience with protein expression and purification methods is also required for most projects. For some projects molecular biology know-how is beneficial, for others experience in protein-DNA interactions and for yet others knowledge of membrane protein crystallization would be a tremendous advantage. Please address applications including the full addresses, fax and telephone numbers of three references to: Wim G.J. Hol, Professor of Biological Structure and Biochemistry, HHMI investigator, Box 357742, University of Washington, Seattle, WA 98195, FAX: 206-685-7002. E-mail: bmsc@goudu.bmsc.washington.edu.



*Meetings were a little more formal in the "olden" days - this photo (courtesy of Hugo Steinfink) was taken at the second ACA Meeting in New Hampton, New Hampshire, August 21, 1950*



*ACA Past Presidents gather at McMaster in 1986*

*Back row: Dave Sayre, Bob Newnham, Dave Shoemaker, and Ken Trueblood. Center row: Ray Young, Jerome Karle, Phil Coppens, Bill Busing, Bill Duax, and John Kasper. Front row: Isabella Karle, Sidney Abrahams, David Harker and Hal Wyckoff.*

**Presidential Memories**

**Elizabeth Wood (ACA President - 1957)**

Rob Burbank's excellent letter covers much that I had remembered. He and I met at a meeting of the American Society for X-ray and Electron Diffraction in 1948 and have kept in touch ever since. That society was so small that the members all knew each other. We met at such places as Gibson Island and a small hotel on Lake George and enjoyed outdoor recreation together.

When it became apparent that ASXRED and the



Crystallographic Society of America were covering much the same ground at their meetings a decision was made to join in a single society. The name American Crystallographic Society was favored by many, but the initials ACS already meant American Chemical Society to most. Bert Warren said that he was a physicist and wanted to keep the name ASXRED with reference to crystals.

When the name American Crystallographic Association was finally chosen Lindo Patterson and I drew up the constitution and by-laws. Contrary to the ruling in many societies, we required two nominations for each office.

In 1956 Jose Donnay who had been Vice-President the previous year became President and I was elected Vice-President, succeeding to the office of President in 1957, being the first woman to hold that office. In that same year I was Chairman of the USA delegation to the International Union of crystallography. This involved a meeting at the State Department in which I shocked them by saying that our delegation would not take instructions as to how to vote concerning the admission of delegates to the IUCr from countries currently out of favor with our State Department.

That was a busy and interesting year for me and I still appreciate the support given me by Bell Laboratories, now included in Lucent Technologies.

### *John S. Kasper (ACA President - 1967) / Charly's Lucht Kasper*



*David Harker  
(ASXRED  
President 1946) and  
John Kasper  
discussing  
inequalities in  
Hawaii in 1979*

John and I wish to thank you for your invitation for him to attend the 50<sup>th</sup> Anniversary Meeting of the ACA in St. Paul. We regret it is not possible for us to attend. John has been legally blind for many years and suffered a stroke 3 years ago that left him able to walk around, but his mind was not so lucky. His memory is very poor and he has trouble finding words to communicate. He knows he was once president of ACA but his memory of that year (1967) is gone. He does not have the strength to travel. The end of March he had a second melanoma removed from his eye and is still recovering from that surgery.

50 years! I joined the ASXRED while a graduate student with Lawrence Brockway when the meeting was held in Ann Arbor in 1943. David Harker attended that meeting and I was offered a good research job at the GE Research Laboratory. . but they would not hire a woman Ph.D. Brockway encouraged me to take the job and finish working for my Ph.D. after the war. I went to

work at GE in February 1944. David Harker was John's Ph.D. (1941) advisor at Johns Hopkins University. When the war was over, he asked John to join his crystallography group at GE.

When the structure of decaborane project began, I worked with the two of them, at first to help with the endless calculations with Beevers and Lipson strips and a Marchant calculator. We soon discovered those calculations could be done with punched cards on the new Research Lab computer. However, using every possible technique then available for locating a few atoms in the structure, we were always stymied by the phase problem. Until the Monday morning when John asked me to see that he could work uninterrupted getting down on paper the ideas he had mulled over all weekend for using Cauchy Inequalities. He thought there was some relationship that could let us fix a few signs (+ or -) and perhaps start to unravel the structure. Dave Harker came in a while later and there was great excitement when he saw that John had indeed discovered a possible way out of our impasse. The rest is history. John presented the paper at the Ste. Marguerite meeting of the ASXRED (by Harker, Kasper and Lucht). The third name was mine. GE was changing the management of the Research Laboratory and they didn't really appreciate what John and Dave had done to solve the phase problem. No time to pursue and refine the math of the phase problem. Jerry Karle was definitely interested and came to visit at GE to go over all the details. Then he and Herb Hauptman went on to develop the direct methods which won them the Nobel Prize.

Dave Harker left GE to work on solving a protein structure at Brooklyn Poly. All of us became charter members of ACA. In 1951 the 2<sup>nd</sup> IUCr was to be held in Stockholm in June. GE approved John's trip to Stockholm and to visit crystallography labs all over Europe as they were recovering from World War II. John and I decided to get married in March so that we could make the trip together. However, GE would not let me continue working at the laboratory as John's wife - so that was the end of my scientific career and the beginning of a long, happy marriage started off with that incredible 6 week tour of European Labs as a slightly delayed honeymoon. I happily entertained all visiting crystallographers who came to GE in subsequent years and attended many ACA and IUCr meetings. Our whole family (3 children) remembers the 1964 meeting at Bozeman. There were 400 accompanying family members at that meeting. The older children helped look after the younger ones. Everyone stayed in the dormitories and wore meal tickets to eat at the college cafeteria. Many long lasting friendships began among the parents as we juggled scientific sessions and kids. The February ACA meetings became my annual vacation when we hired a housekeeper to care for the children, and we went to Seattle, Tucson, New Orleans, Atlanta, Charlottesville and Hawaii. The 1977 meeting at Asilomar we took our 16 year old younger son. Bob played golf most of the time, but has never forgotten Brockway claiming him as a scientific grandson, and Pauling (the Banquet speaker) shook his hand and said that made him his great grandson. Bob is now a college professor and still takes his Vitamin C! And he said it really made him appreciate his studies of Chemistry and Physics to have met over the years so many of

the men and women he was reading about. When John was president of ACA, I sat next to Sir Lawrence Bragg at dinner. We had met on several previous occasions in Europe. We both attended the Buffalo meeting of the ACA Sid Abrahams wrote about in his letter. In 1969 most of the arrangements for the IUCr VIII meeting at Stony Brook had to be made by John since David Shoemaker was in Europe. The caterer at the clam bake on Fire Island insisted that in order to be sure he collected every ticket, all 2000 people should wait in line single file to get their traditional bag of food. A sight never to be forgotten. John finally argued him into several parallel lines. Then the French complained that it was barbaric to sit in the blowing sand to eat something as elegant as a lobster!

Sidney Abrahams hoped that the copy of his letter he sent to us would help John's memory - unfortunately it didn't. I have tried to add some of the personal things that happened over the years, and to mention some of the problems that women scientist faced.

Even giant companies have had to change their policies with the times. When John retired in 1980, they hired Dr. Mary Garbaskas to continue the X-ray crystallographic research and she was just one of many women with PhD's working there.

We are certain that the 50<sup>th</sup> Anniversary Meeting will be a great success and regret that we will not be there to see old friends and appreciate all the scientific progress that has occurred since ACA began.

### *Sidney C. Abrahams (ACA President - 1968)*

**Recollections of the ACA at Penn State, Tucson & Buffalo 1968:** Ralph Wyckoff, second president of the ACA, told the Tucson meeting in 1968 that "he was struck by the lack of a sense of history, not only in the outlook of students but in the way science is taught." He went on to say that we should realize we live in a moment of time with important characteristics set by all that has gone before and that we can only perceive the real meaning of our efforts if we appreciate how we come to be making them. The present recollections are not the place for such an overview, beneficial as they might be. Instead they offer brief looks at the 1968 period, when it was my privilege to serve as ACA president, at our first meeting in 1950, and at our most recent meeting in Buffalo as a comparison in miniature.

The ACA had 495 charter members and annual dues of \$5.00 in 1950, with Isidor Fankuchen (Fan) as our first President. A total of 120 members participated in our first meeting at Penn State, with ten sessions spread over three days. There were few, if any, accompanying members. The meeting immediately followed a Conference on Computing Methods and the Phase Problem at which David Sayre, later to be 34<sup>th</sup> ACA president, demonstrated the existence of simple connections between structure factor signs. Ferment in this area had started three years earlier with the discovery by David Harker, 6<sup>th</sup> president of ASXRED and John Kasper, 18<sup>th</sup> president of ACA, of structure factor inequality relationships. Ray Pepinsky's analog computer,

that instantly let us produce contour maps from a bank of sine wave generators, was also of great interest at this meeting. With amplitudes and phase angles (0 or 180°) set by dials and switches on each generator rack, many trial models could be examined in short order; use of this unprecedented capability brought many of the world's leading crystallographers to Penn State. In addition to a general interest in computers, no doubt related to a distaste for the manual calculations we all performed then on the ubiquitous Marchant or Monroe calculating machine, and in the phase problem, there was considerable activity in developing a range of new techniques.



*Walter Hamilton (President - 1969), Sidney Abrahams (President - 1968) and John Kasper (President - 1967)*

Among them were methods for extending diffraction measurements to subambient temperatures. Fan had started this approach a year or two earlier with a directed cold air stream that cooled a crystal mounted on a precession camera. I had the opportunity the previous year, on my way to Minneapolis as Bill Lipscomb's (ACA's 6<sup>th</sup> president) first post doc, of seeing Fan's initial experimental technique. We recognized it as an important advance and were able to improve it, as Fan did also, to become a routine tool from which cryogenic crystallography grew. The majority of the papers at Penn State presented the structures of small organic molecules and simple inorganic materials. All x-ray single crystal diffraction records at that time were registered photographically, and nearly all calculations were made manually. Nevertheless, the meeting had an atmosphere of intellectual excitement and confidence that we would meet the challenges of our field. It was also notable for the generous personal level of interaction among the participants, among whom were such major figures in our field as Lindo Patterson, Bert Warren, Martin Buerger, Paul Ewald and Willie Zachariasen.

The ACA thenceforth met twice yearly until 1984, except for every third year when an IUCr Congress was held. The tradition of scheduling spring meetings in the South and summer meetings in the North made the ACA very accessible to graduate students and faculty around the country. We almost always met on a university campus at no charge. Registration fees were low but paid most of the meeting costs, primarily that of printing and mailing the Abstracts, and most members were willing to use dormitory accommodation. Many lasting personal friendships developed during these meetings.

The spring meeting of my presidency was held February 1968 at Tucson, the summer meeting in August at Buffalo. John Kasper was immediate past president, the ACA having met the previous January at Atlanta and in August at Minneapolis. Walter Hamilton was president when the ACA met March 1969 in Seattle and the Eighth IUCr Congress convened in August at Stony Brook. The accompanying photograph shows these three presidential friends at the Buffalo meeting picnic on Goat Island.

ACA membership had increased to 1,650 by 1968, the annual dues to \$10.00. Tucson attracted 330 participants with 84 papers presented over 14 sessions, while Buffalo drew 480 participants with 150 papers over 20 sessions. Both had registration fees of \$8.00. The meeting in summer was always larger than in spring. As was common in those days, ACA Council met all day Sunday before the scientific sessions began, adjourning in time for the traditional evening social to welcome the meeting participants. Among its actions was a proposal for presentation to the Business Meeting later that week by which Council members would automatically become members of the USNCCr, following its earlier reciprocal action. Council also met next evening with the National Committee under chairman David Shoemaker, our 21<sup>st</sup> ACA president; the deliberations largely concerned local arrangements for the forthcoming IUCr Congress since the National Committee was financially responsible. The writer succeeded David the year following the Congress, thereby inheriting the task of winding up its fiscal obligations. Fortunately, the earlier rather gloomy financial predictions gradually improved and the final balance provided the USNCCr with substantial reserves that allowed it to support young crystallographers in attending future Congresses.

The state of crystallography by the time of the Tucson and Buffalo meetings had advanced strongly since Penn State. Scintillation counters had largely replaced film for recording x-ray diffraction by single crystals, and the automation introduced earlier in the decade had been incorporated into several commercially available automatic diffractometers. A major concern was the accuracy of these instruments, see Volume 1 of the ACA's *Transactions* for an interesting discussion. Nearly all computations by 1968 were made on mainframe computers or on an increasingly popular series of minicomputers used also to control the diffractometer. Direct methods for solving crystal structures had come into routine use, particularly for organic and biological molecules.

The program in Tucson was rather evenly balanced, with about one-fifth of all papers devoted to organic and biological molecules and the same to inorganic materials; the remainder was distributed about equally between the symposium topic of low energy electron diffraction and thermal motion, the physics of solids and surfaces, apparatus, and diffraction theory.

In a change that foreshadowed a continuing trend over the subsequent decades, more than one-third of all papers presented at the 1968 Buffalo meeting were concerned with biological structure, about one-quarter with organic and organometallic structures, one-fifth with inorganic and mineral structures and the remainder distributed among small angle scattering, the

physics of x-ray diffraction, dislocations and defect structure. There were 81 registered accompanying members, with an unrecorded but substantial number of children present, reflecting a lifestyle now largely vanished; comparable numbers were found at ACA meetings during most of the 60's and 70's.

In comparing the 1950 and 1968 meeting statistics with today's, we must use those from 1999 since this year's are still incomplete. ACA membership last year was 2473, with annual dues of \$75.00; membership peaked at 2597 in 1995. Buffalo in 1999 drew 632 registrants with a registration fee of \$225.00. 339 papers were presented in 32 sessions over 6 days, about 75 % of the papers being concerned with biological structure.

A much fuller account of the background leading to the ACA's formation and its subsequent development may be found in *Crystallography in North America* (1983), edited by Dan McLachlan, Jr. & Jenny P. Glusker, and published by the ACA. It was a valuable resource for these recollections. A companion edition bridging the period between 1982 and our 50<sup>th</sup> anniversary would provide priceless information for the society when it approaches its 75<sup>th</sup> and later anniversaries.

It is a pleasure to thank Marcia Evans, ACA Administrative Manager, for her kind search of the archives resulting in many of the statistics given here.

### *Bill Busing (ACA President - 1971)*



*Henry Levy (ACA President - 1965) and Bill Busing in 1956, a time when their least-squares refinement program ORFLS was THE program for refining crystal structures.*

My recollections don't go as far back as Rob Burbank's, but I do remember my first ACA meeting at French Lick, IN, in 1956. At that meeting Joan Clark reported on what I believe was the first crystal structure determined entirely by direct methods. (I think the authors were Clark and Crist and perhaps Howard Evans. At this point I don't have the facilities to look it up.) Someone, probably Ray Pepinsky, asked what the Patterson map looked like, and when Joan said they hadn't made a Patterson, there was a general gasp of surprise.

As President I remember the 1971 meeting in Charleston, SC. One of the presidential duties that I did not particularly like was being responsible for the protocol at the banquet. Fortunately I

had Julie Roth, Secretary Walter Roth's wife, to advise me about seating at the head table. Martin Buerger was there to receive the first Fankuchen Award and Dina Fankuchen was there also. I remember having to intervene when an overly conscientious waiter tried to extract a banquet ticket from the university Vice President. Ben Post gave the banquet address. His topic seemed to be that, while everybody else was interested in information retrieval, he was more interested in information disposal. Imagine what he would have thought about the internet and junk mail!

### *Jerome Karle (ACA President - 1972)*

### *Isabella Karle (ACA President - 1976)*

**Fifty years plus:** We became familiar with the electron diffraction and X-ray diffraction communities during the 1940s. There was at least one meeting of the Crystallographic Society of America at the University of Michigan during the 1944-46 period. Isabella was there during that period as a member of the chemistry faculty and Jerome was employed there by the Naval Research Laboratory on a World War II project. This was when we first met Martin Buerger and Lindo Patterson. David Harker, Jose Donnay, William Zachariasen and Isidor Fankuchen were also there. There were additional meetings of the Crystallographic Society of America and also meetings of the newer society called The American Society for X-Ray and Electron Diffraction (ASXED) until 1950 when the American Crystallographic Association was formed from a merging of the above two organizations. After the war, Paul Ewald joined Fankuchen at the Polytechnic Institute of Brooklyn and added his presence to the meetings. Our thesis professor, Lawrence Brockway, a major figure in gas electron diffraction, was also an attendee at the meetings.

The gentlemen listed were the leaders with whom we had the most contact. They were very friendly to young people, respected each others competence and maintained the dignity of their profession. We miss their presence. There were other distinguished leaders, but we had only passing contact with them.

In 1948, the first meeting of the International Union of Crystallography took place at Harvard University. Lindo Patterson invited us to join him, Paul Ewald and Max von Laue at their dinner table. We had very pleasant and interesting conversations with those gentlemen.

Our experiences as Presidents of the ACA were quite standard. There were the usual arrangements to be made for meetings and for the other activities associated with maintaining the organization. In this connection, we would like to mention the dedicated efforts of Ray Young (Robert A. Young) to ensure that the venues for the meetings were optimal in terms of expenses and the convenience of attendees. Ray did this for several years.

We have a suggestion concerning meetings. Over many years, oral presentations were chosen after abstracts were submitted. We have the impression that decisions concerning oral

presentations are made now within special interest groups without soliciting the suggestions of the members via abstracts. If this is the case, the defects of such a system dictate the necessity for change.

### *Robinson Burbank (ACA President - 1975)*



I was pleased to read in the Winter 1999 Newsletter of plans to celebrate the 50th anniversary of the ACA. I well remember some of the history behind this anniversary.

In January, 1948 I joined the American Society for X-ray and Electron Diffraction at the instigation of my friend and colleague Howard Evans. In March, 1948 I attended my first ASXRED meeting at Yale. The business meeting the planning was started for the scientific program for the first IUCr Congress coming up at Harvard later that summer. Can you imagine such a thing being contemplated today based on a lead time of barely four months? Life was simpler then and everything came out on schedule. Three Nobel Laureates attended the meeting. Peter Debye and Sir Chandrasekar Raman were lively and unpredictable participants in the technical sessions while Max Von Laue was elected honorary president of the IUCr. During the meeting informal talks were commenced between representatives of the ASXRED and the Crystallographic Society of America about combining their memberships into a single new society. These preliminary talks ultimately solidified into specific proposals following vigorous and sometimes acrimonious council meetings and business meetings of both societies in 1948 and 1949. In September, 1949 ballots for voting on the dissolution of the existing societies, a constitution for the new society, a choice of name for the society, and membership applications were distributed to the memberships. By a margin of over 10/1 the vote was for a new society. By a much smaller margin the favored name was the American Crystallographic Association. Thus, on January 1, 1950 the ASXRED and CSA ceased to exist and the ACA was born. Approximately 470 applicants became charter member of the ACA. It would be interesting if the society records can indicate how many of those charter members of more than 50 years ago are still ACA members today.

At the first ACA meeting held at Penn State in April, 1950 by far the principal attraction was Ray Pepinsky's X-RAC analogue computer. It performed the same functions as the Beever-Lipson strips but the effect of adding each reflection and varying its phase could be seen immediately on an oscilloscope screen. There was a six foot tall electronic rack for each Miller index and the net result was a very large room completely filled with electronic racks and a prodigious number of vacuum tubes. Ray had a full time, and very temperamental technician who had to replace the tubes as they burned out to keep things running. For several years an international clientele of crystallographers made pilgrimages to Penn State with their data until the digital computer revolution caught up with and made the analogue approach

obsolete.

Twenty five years ago in 1975 most of our founding fathers were still alive and many of our past presidents came to our 25<sup>th</sup> anniversary observance at the University of Virginia in March. At the banquet they were introduced in reverse order of seniority concluding with Maurice Huggins who had been the first ASXRED president in 1941. My esteemed friend Betty Wood gave an address about the early days which was so memorable and evocative that it elicited a much deserved standing ovation at its conclusion. All in all it was a happy and sentimental occasion.

In the ensuing 25 years crystallography has evolved in ways quite beyond my imagination and competence except to note that they exceed our wildest dreams of those earlier times. The Good Lord willing I will endeavor to attend the 50<sup>th</sup> anniversary banquet this coming July 26<sup>th</sup>.

### Jenny P. Glusker (ACA President - 1979)



I first came to the US in September 1955 as a postdoc with Bob Corey at Caltech and then came East the next year (by car, missing the French Lick meeting) to Philadelphia to work with Lindo Patterson. As a result, my first American meeting was the IUCr meeting in Montreal, Canada, in 1957. What a wonderful meeting that was, and my best memories are of the day-long boat trip in which one could meet everyone on board, and the visit to the St. Lawrence Seaway construction (where I met Isidor Fankuchen). At the fall ACA meeting at the Mellon Institute I met Vladimir Vand. So, for me, the early ACA meetings were important because I could meet and talk with the crystallographers that I knew about only from their scientific articles and books.

In 1979, when I was President of ACA, there were two ACA meetings, one in Honolulu, Hawaii in March (at the University of Hawaii, just before the American Chemical Society meeting in the same city), and in Boston (at Boston University) in August. Before the meeting in Honolulu there had been a meeting on "Modulated Structures," suggested and organized by Carroll Johnson, at the King Kamehameha Hotel at Kailua Kona on the island of Hawaii. The Hawaii meeting, joint between the US, Japan and China, was the idea of Philip Coppens, the previous ACA President. It was my job to invite some Chinese crystallographers to the ACA meeting. This was not easy. The US did not have a Chinese Embassy in Washington in those days, only a Liaison Office. Letters to China went unanswered until I sent one in Chinese (with a covering letter explaining what I thought the letter said). Then came the reply that two Chinese crystallographers would attend, and Professor You-chi Tang was able to give a talk on the state of crystallography in China at that time. He asked me why I sent a letter in Chinese when he could read English. The opening of the ACA meeting was spectacular because the power failed throughout the entire university campus as I was introducing speakers in the Opening Ceremony, but it was restored in about half an hour. The other problem was a

strike by United Airlines that left many on the island for longer than they had intended, but none were permanently stranded and some had interesting journeys home. However, we had Hawaiian dancing at the banquet with Linus Pauling as an honored guest.

The summer meeting in Boston concentrated on macromolecular crystallography, a subject that had not been well represented in some of the previous ACA meetings. Martha Ludwig arranged a magnificent program; for example, it included one of the first reports on Z-DNA (from its home base in Alex Rich's lab). The Warren Award, attended by Bert Warren, was given to Drs. Lytle, Sayers and Stern for their EXAFS work.

The science of crystallography has progressed rapidly through the last 50 years, and the memories of the people involved, their introduction of new ideas by scientific presentations at meetings and their friendly interactions with other scientists, young and old, have made the ACA the subject of great pride for all of us.

### David Sayre (ACA President - 1983)



**SOME REMINISCENCES:** It was my good fortune, one day in 1947, when I was a graduate student at Harvard and very unsure of what I wanted to do, to come across the wartime review article on x-ray crystallography, in the Annual Reports on Progress in Physics of the Physical Society of London, by J.M. Robertson in Glasgow.

Here I was, looking at a molecule (platinum phthalocyanine), and "seeing" every atom in it! In that instant I knew what I wanted to do, and in 53 more years the excitement has never worn off.

The next year, now a member of Ray Pepinsky's group in Auburn Alabama, I attended my first crystallographic meeting, the March 1948 ASXRED meeting described in these reminiscences by Robinson Burbank; it was at that meeting that the plans for the ACA were made. Here are my memories of it, written recently as part of some personal reminiscences:

"Another important part of my Auburn experience was that of beginning to become acquainted with the crystallographers of America and the world. This was something in which Ray acted very thoughtfully and generously in our behalf. In March 1948 a small delegation of us from Auburn travelled to Yale to take part in what was for me my first crystallographic meeting, and there I could see and listen to most of the notable American crystallographers: from Bryn Mawr, A.L. Patterson himself; from Brooklyn Polytechnic, Isidor Fankuchen; from MIT, Martin Buerger and Bert Warren; from Johns Hopkins, Jose Donnay; from the University of Chicago, William Zachariasen; from Cal Tech, Linus Pauling, Eddie Hughes, and Verner Schomaker; to name only a few of the best-known of the perhaps 50 persons there. I was struck on this occasion by what I never failed to be struck by again and again through the years: the extraordinarily high technical and human quality found in this small field of science. In those days, with no need for parallel or poster sessions, every paper was spoken, and heard with attentiveness. At the end of the paper, someone (usually one of the senior group)

would comment unhurriedly and informatively on what we had heard; someone else would speak; and serious general discussion and give-and-take would follow. These were old friends, who knew and loved their subject, and valued one another's opinions."

(From Rob Burbank, by the way, I learn how imperfect my memory is in some ways. There were actually 205 crystallographers present, and Pauling did not attend, though Jerry Donahue was present and spoke.)

Also in the summer of 1948 I attended the 1st IUCr Congress which took place at Harvard. Rob refers to Sir Chandrasekar Raman as one of the notables at that meeting, and describes them as being gifted with unpredictability. How true! Raman's talk was on the structure of diamonds, and partway through his talk he reached absent-mindedly into his pocket, took out a diamond about the size of a pigeon's egg and tossed it idly from hand to hand for the remainder of his talk. You may be sure that every eye was on him.

My year as president of the ACA was 1983, following Jerry Cohen and being followed by David Templeton. Our 1983 meetings were in Columbia, Missouri and Snowmass, Colorado. At that time Council's major concern was that crystallography might find itself drifting into being a technique only, and thus in danger of becoming a second-order participant in the sciences to which it would be contributing; to that end we sought to identify the ACA with a higher concept of how our subject might operate in science. That effort I think has been continuously maintained in the ACA, and when I look at the work being done by crystallographers today I feel that the danger has truly been averted.

Our 1984 meeting was in Lexington, Kentucky, where following tradition I had to give the past-presidential talk. I expect that my talk has been pretty well forgotten, but I know there are many who still remember the talk about Rosalind Franklin which my wife Anne gave at that meeting. Anne is gone now, having died in March 1998, and I will never cease to be grateful that the ACA asked me to provide an obituary of her for inclusion in the ACA Newsletter. Although Anne was not a scientist, she loved and understood the caring which crystallographers give to each other and to their subject, and being herself included in that caring by the ACA would have moved her deeply.

As I look back over the last 53 years, I see a subject — initially small but beautiful, deeply contributive to science, and lovingly practiced — continuing its development amazingly further, and doing so in a manner still true to its origins. The work in which I have been engaged in recent years convinces me that when we have run out of crystals there will still exist almost limitless areas for continued growth. I feel deeply fortunate that this beautiful field has been a major part of my life.

*In 1950 ACA dues were  
\$5.00 for regular members  
\$3.00 for students*

### **Bill Duax (ACA - President 1986)**

Some people have accused me of installing myself as ACA President for life and I appreciate the fact that so many ACA Presidents have been tolerant of my often meddlesome presence. I'm sorry, I just can't help myself. Crystallography seems to be my *raison d'être*. The beauty of the discipline and the people it attracts continues to enrich my life to an extraordinary degree. When I think of my life in the ACA I see a flood of images. At my first meeting after my first talk David Harker spoke a kind word to me. At the time I didn't recognize him and my thesis advisor Norman Baenzinger had to tell me that it was the David Harker that I read about in text books. I learned that "kind words" were not what David was most famous for at ACA meetings. A few years later I was puzzled when David stood up in the audience at the annual meeting and berated a couple of speakers for not understanding the principal of homometric solutions (the speakers were a couple of whipper snappers named Karle and Hauptman). A few years later when I suggested that the ACA start holding only one meeting a year, I vividly recall Sidney Abrahams telling the attendees at the business meeting that "if Bill Duax doesn't like coming to two ACA meetings a year he doesn't need to come to ACA meetings at all". Smarting from the remark (I always took things too personally) I was tempted to leave the ACA but Jenny Glusker (ever my good angel) persuaded me that Sidney meant no harm. Jenny was almost always right. A few years later Jenny talked me into being a write-in candidate for ACA president, perhaps the only occasion in which a write-in candidate appeared on a ballot. As a consequence the ACA office had to hold a run-off election, wasting paper and postage to elect one of the original candidates.



### **Bill and the Gorilla - ACA Banquet 1987**

When I was elected president in 1986 the annual meeting was held at McMaster University in Hamilton, Ontario, Canada. The local chair I. David Brown and program chair Martha Teeter did a wonderful job. It was the first meeting after the announcement of Hauptman and Karle's Nobel Prize in Chemistry and Robert Bryan masterfully chaired a session in which he said that the H, K, and L of crystallography were the sessions speakers (Hauptman, Karle and Linus). Jane Griffin chaired the transaction symposium on Hydrogen Bonds that year and we broke tradition and presented the Fankuchen award on the last day of the meeting rather than the opening session to accommodate the hectic schedule of Michael Rossman who mesmerized the audience with his lecture of a spherical RNA virus. A wonderful memory from my past president years was having Dorothy Hodgkin present at the

Austin meeting to present the first Pauling Prize awards to young crystallographers at the dinner. At the same dinner someone in a gorilla suit sent by the “women of crystallography” delivered a bouquet of balloons to me and I finished my past president talk by somersaulting down the center of the banquet hall. The Philadelphia meeting in 1988 was another high water mark in my memory. The presence of six Nobel Laureates (Hodgkin, Pauling, Lipscomb, Hauptman, Karle and Kendrew) drew an attendance of nearly twice that of previous year.



**Bill Lipscomb (ACA President - 1955) explaining x-ray crystallography to Ben Franklin at the ACA Banquet in Philadelphia 1988**

If anyone wants to know who to blame for saddling the ACA with me as a volunteer CEO, the guilty party is Catherine Foris who not only served as a splendid treasurer but paved the way for the election of her successor Rao. During my year as president the ACA office was transferred to Buffalo and a new era began. The ACA office began in Buffalo with the help of Debbie Savage and has continued to grow and serve the expanding needs of the membership under the capable direction of the marvelous Marcia Evans and her staff. While the ACA continues to thrive due to the volunteer efforts of a great many individuals as officers, program and local chairs of the annual meetings and editors of its newsletters, the value of an office with a full time staff has become abundantly clear. The importance of the powerful discipline of crystallography to the infrastructure of science requires a support structure equal to the task of serving the science and its practitioners. A 50th anniversary meeting might be a good place to gather and discuss the future of the ACA.

**Charles E. Bugg (ACA President - 1987)**



Thank you very much for your letter informing me of the get-together for the past ACA presidents at the meeting this summer in St. Paul. I am planning on attending the banquet on the evening of Wednesday, July 26, and I will be looking forward to seeing you and many of my other friends who have served the ACA with such enthusiasm over the years.

My main impression of crystallography during my brief career is WOW! I feel extremely fortunate to have been in this exciting field during two major revolutions in the field of crystal structure analysis, first in small molecule crystallography during the 1970's, and then in protein crystallography during the 1990's. As a graduate student during the early 1960's, my Ph.D. thesis involved solving the crystal structures of two extremely small

organic molecules, which I considered a major accomplishment at the time. Clearly, this would take well under a week with today's techniques. At about the time that I was President of the ACA, we enjoyed a similar transition point in protein crystallography, as the Protein Data Bank began its sharp transition from flat growth to the exponential growth that we have today.

I feel equally fortunate to be participating now in another revolution in applications of crystallography, including development of more and more effective ways of using the power of crystallography in the design of unique pharmaceuticals that are addressing many major medical problems. Hopefully, I am still young enough to see a couple of additional revolutions occur using our very powerful science before they put me in the grave!

Many thanks to you and to the ACA for organizing this wonderful opportunity for us to get together in St. Paul. I'll see you there.

**Helen M. Berman (ACA President - 1988)**

**ACA memories:** The ACA is a very special organization that provides vehicles for learning about the latest developments in crystallography, watching the field evolve, and making friends that can last a lifetime. I feel lucky that I became involved with it at an early stage of my career having attended my first meeting in 1965 while still a student at the University of Pittsburgh. When I gave my first talk I remember how happy I was when Lindo Patterson asked me a question. I also remember the meeting in Atlanta when the first “American” protein crystal structure-ribonuclease was described.



**Ned Seeman, Joel Sussman, Helen Berman and Sung Ho Kim holding early discussions about the PDB**

*Handwritten list of names and affiliations, including: E.L.M. Group, Director Biochemistry, University of Tennessee, Knoxville; H.A. Schell, Dept. of Chemistry, Yeshiva Univ., New York; J.R.P. Searl, Dept. of Chemistry, University of Toronto; Srinivasan, Institute of Biological Sciences, University of Madras; Helen, Boston, MA; Donald, West; James, University of California; Fred, Boston, MA; David, Iowa; Council of Chemists; Ed, Johns Hopkins; Walter, E. Lewis; PDB Committee; W. Gary Thornton; J.D. May; Robert, University of Virginia; Jim, Johns Hopkins; and David, Johns Hopkins.*

*Part of the original petition to start the PDB that was submitted to the ACA.*

In 1971 when I was not yet 30 and had been going to ACA meetings for six years, I began to realize that those meetings could be an important forum for “making important things happen”. I got together with a group of like-minded colleagues and we had a grass roots meeting to encourage the ACA to help establish a protein data bank. We had a meeting in Columbia, South Carolina and many people signed a petition endorsing such an effort. After the PDB was in fact established at Brookhaven, the ACA did indeed give it its sponsorship (unfunded of course) and for many years the PDB sent regular reports to the ACA.

In those early years the young folks including myself, Bill Duax, and Judy Flippen-Anderson among others were full of new ideas that eventually became part of the mainstream. We came faithfully to the business meetings where we argued our causes and occasionally even won. Notable successes were the establishment of poster sessions (complete with beer), once a year meetings (rather than two), SIGS, and Continuing Education Workshops.

Eventually we all turned 40 and became part of the establishment. This earned us the right to be in charge of things. And so in 1987 I had the honor of being Program Chair for the Austin meeting. In addition to organizing the scientific content of the program, we had to cut and paste (with scissors and glue) the abstracts onto big layout sheets so that they could be photographed for inclusion in the Abstract book. This was an exhausting task and I was lucky that Judy came up to Philadelphia to help after I convinced her that this was good training for when she would be a Program Chair the next year.

Then in 1988 I presided over the Philadelphia meeting as President of the ACA which was attended by a record number of people including a pretty good facsimile of Benjamin Franklin.



*Michael Woolfson, Helen (with feathered friend), and Dave Duchamp at the ACA banquet in New Orleans - 1990.*

For logistical reasons, I did not get to give my Past President’s speech at the 1989 Seattle meeting and so Bryan Craven had me give it in 1990 in New Orleans (thereby missing his chance to do this dreaded duty). Afterwards Bill Duax decided to present me with a series of honors including a pink feather boa and some other unmentionable prizes

Once I finished with my ACA Council duties, I found myself in new projects. I worked with Paula Fitzgerald who patiently and courageously led the creation of the mmCIF dictionary- a project that we thought would take a weekend and took almost eight years. But there were rewards; among those were that we got to eat in lots of neat restaurants and we were mostly right about which ones would last.



*George Jeffrey, Ben Franklin and Helen at the ACA banquet in Philadelphia - 1988.*

Being part of the ACA for 35 years has been fun, hard work, and often times rewarding. I learned a lot of new science by attending talks and posters. I also learned about the interplay of community and science that has been invaluable for my present responsibilities directing the PDB.

*I would like to include more ACA memories in upcoming Newsletters. If you have old photos or memories to share, please send them to Judy Flippen-Anderson, [flippen@harker.nrl.navy.mil](mailto:flippen@harker.nrl.navy.mil)*

## ACA Commercial Exhibits

The ACA exhibitors have been part of our meetings since the very beginning. I wrote to a number of our current, and past, exhibitors asking for historical artifacts and anecdotes. Unfortunately, many of the folks currently involved were not around in the "good old days" so the historical stuff has not been easy to find. I'm including what I did get. However, I wasn't always sure who to contact so if I missed anyone or if someone is still out there from the earlier, or more recent, days of our exhibits please be assured that we will be happy to include more in the remaining issues of the Y2K edition of the Newsletter. The ACA is 50 all year long, so any of our commercial friends are welcome to share ACA memories with us after this issue goes to press. I'm grateful to all of you who are willing to search your archives for me.

*Judy Flippen-Anderson*

**From Charles Supper, Inc.** *Lee Supper remembers the 1st ACA meeting in State College PA in April of 1950.* "This meeting was an important event for Charles Supper Company. Dad had never had an opportunity to meet and talk with so many potential customers about his product line of cameras and goniometer heads. He and Mother shared booth duty - as a 12 year old I was the gopher. I remember a few nights of the three of us at our dining room table putting mimeographed descriptions of the products into a cover he had printed for the meeting.

Aside from our little firm, Otto von der Hyde also exhibited. Otto and Dad were friendly competitors, having met in 1924 when they were both entering the United States from Germany. Each was a highly talented instrument maker and they worked together at several jobs before coming to Martin Buerger's machine shop at MIT in the mid/late 1930's. For a time, Otto produced products similar to ours. Phillips and General Electric were represented, possibly Jarrell-Ash and Picker. No others to my recall.

The commercial attendees were located in one room in either an Inn (Nittany Lion?) or a campus house. Each exhibitor had one or two card tables for brochures. It was all very congenial - Otto, who was an accomplished pianist, played a grand piano every night, even getting into popular songs and song fests. Phillips (Jack Washburn) had at least one cocktail party which we know became a Phillips and ACA tradition (I only heard about the party).

These simple arrangements for commercial exhibitors continued for perhaps a dozen years or so. They are greatly missed by this writer."

**Sue Byram (Syntex - Nicolet - Siemens - Bruker)** says that the earliest evidence she can find for exhibiting with the ACA was in Ottawa in 1970. She found some photos that chronicle her professional evolution/metamorphosis! Top photo is a beardless Bob Sparks (circa early 70's); next is Godfrey Crane (mid-70's); then Sue, Omar Lutfey, Rod Cook and Rich Peach (Pittsburgh - 1992) and finally Sue in Arlington, VA (1998).





*Molecular Structure Corporation (MSC) is another long time ACA commercial exhibitor and corporate member. This year marks the 17th anniversary of their annual Fun Run. - the T-shirts were instituted in 1985. The photo shows some very happy (that it's over) runners in 1997 in St. Louis, MO in the memorable tie-dyed T-shirts.*

**From Bert Frenz of B. A. Frenz & Assoc:** "Any photos I may have are buried in a storage unit where we moved all our household possessions about 18 months ago. Since then we have been traveling full-time in our motor home (right now we are at Mammoth Cave National Park, heading to Newfoundland for the summer).

I started on the commercial side of ACA right after my postdoctoral position at Texas A&M and I probably participated in my first commercial exhibit in 1975 when I promoted the SDP software through Enraf-Nonius.

I don't recall any particular stories of the ACA commercial exhibits at that time, but one theme was consistent through the early days of my experiences. It seems that whatever I was promoting was always a bit ahead of the times and not quite accepted. When I promoted running crystallographic software on minicomputers, crystallographers could not envision leaving their mainframes. When I proposed switching from PDP-11 mini-computers to VAX-11 computers, Enraf-Nonius didn't support the move. When I began my work with microcomputers - starting with the IBM-AT - I met many naysayers who were firmly in bed with their VAX computers. And then, even when small molecule crystallographers had adopted minicomputers, their macromolecular counterparts hesitated at my suggestion to leave their workstations for less expensive minicomputers. All of this seems hard to believe now that small personal computers are an everyday part of our lives and crystallographic calculations spin off our notebook computers as fast as arithmetic on a hand calculator in the early 70s."

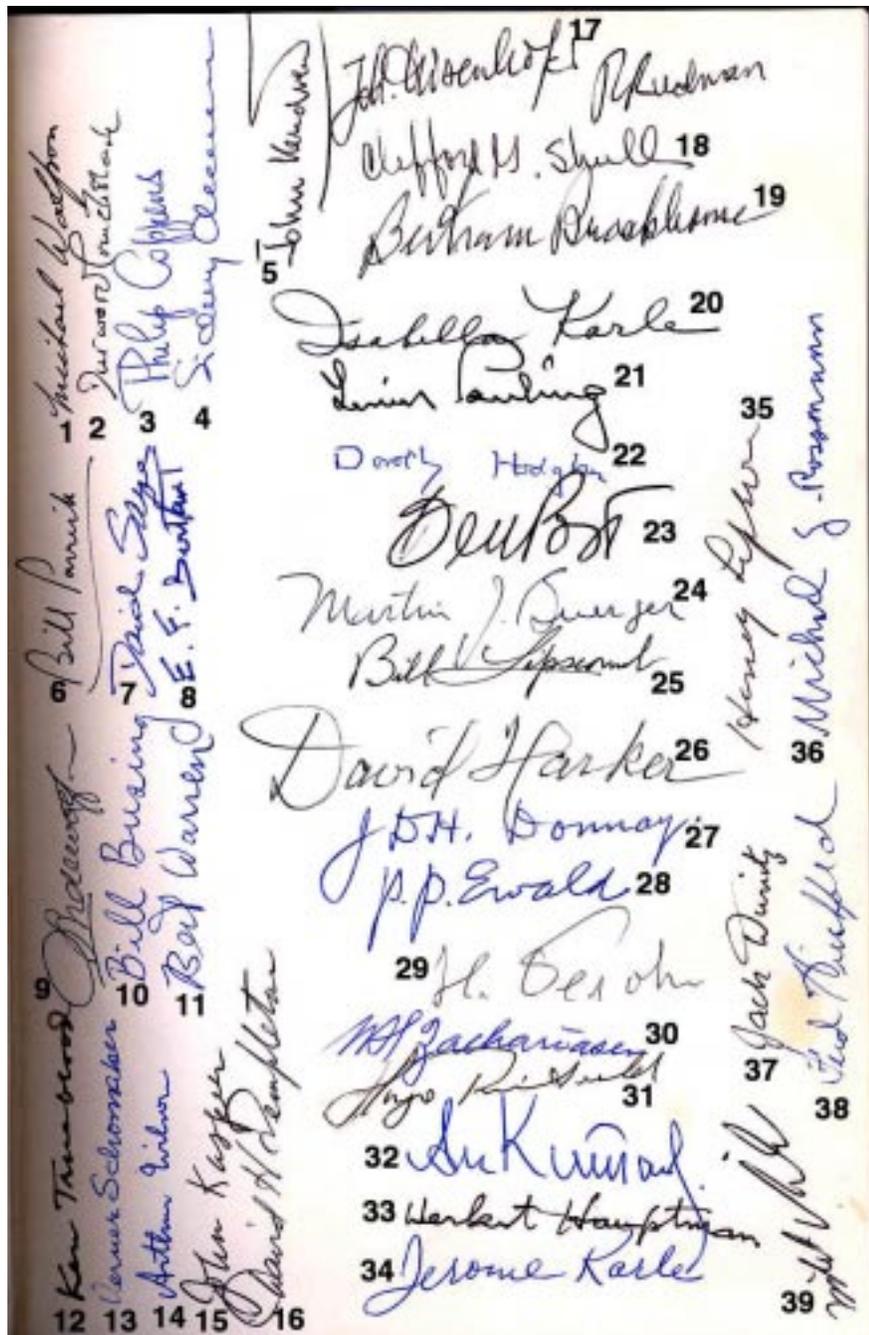
Name that Crystallographer

It was February 1977, the world was young (or at least I was younger), and it was the ACA Meeting at Asilomar, Pacific Grove, California. Linus Pauling was in attendance and Dorothy Hodgkin was the recipient of the Third Fankuchen Award. My book on "Low-Temperature X-Ray

Diffraction: Apparatus and Techniques" had just appeared and I had organized a tutorial on the subject. At one session I had a copy of the book with me and found myself sitting next to Linus Pauling. On the spur of the moment I asked him to autograph the flyleaf of the book, which he graciously did. Later that meeting I asked Dorothy Hodgkin to autograph it too.

Following that auspicious beginning, I began to carry the book with me to various crystallographic meetings. During the past 22 years many of the best known names in crystallography have kindly added their signatures to that page. A copy of the page is printed here for your perusal. How many signatures can you identify? Can you also identify their contributions to our field?

Reuben Rudman



- 1. Michael Woolfson
- 2. Durwood Cruickshank
- 3. Philip Coppins
- 4. Sidney Abrahams
- 5. John Kendrew
- 6. Bill Parrish
- 7. David Sayre
- 8. E. F. Bertaut
- 9. Pieter de Wolff
- 10. Bill Busing
- 11. Bert Warren
- 12. Ken Trueblood
- 13. Verner Schomaker
- 14. Arthur Wilson
- 15. John Kasper
- 16. David Templeton
- 17. H. Diesenhofner
- 18. Clifford Shull
- 19. Bertram Brockhouse
- 20. Isabelle Karle
- 21. Linus Pauling
- 22. Dorothy Hodgkin
- 23. Ben Post
- 24. Martin Burger
- 25. Bill Lipscomb
- 26. David Harker
- 27. J. D. H. Donnay
- 28. P. P. Ewald
- 29. N. Belov
- 30. W. H. Zachariasen
- 31. Hugo Rietveld
- 32. A. I. Kitaigorodsky
- 33. Herbert Hauptman
- 34. Jerome Karle
- 35. Henry Lipson
- 36. Michael Rossmann
- 37. Jack Dunitz
- 38. Fred Hirschfeld
- 39. Hartmut Michel

KEY: