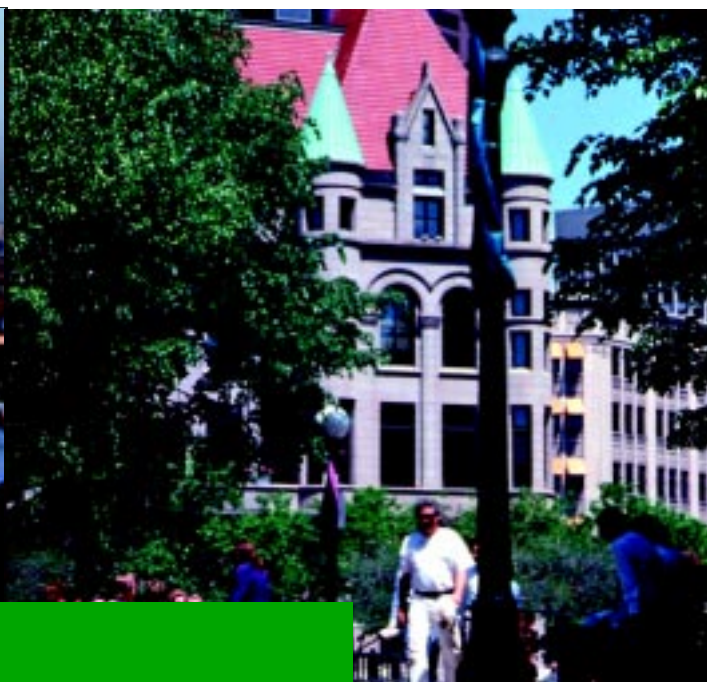
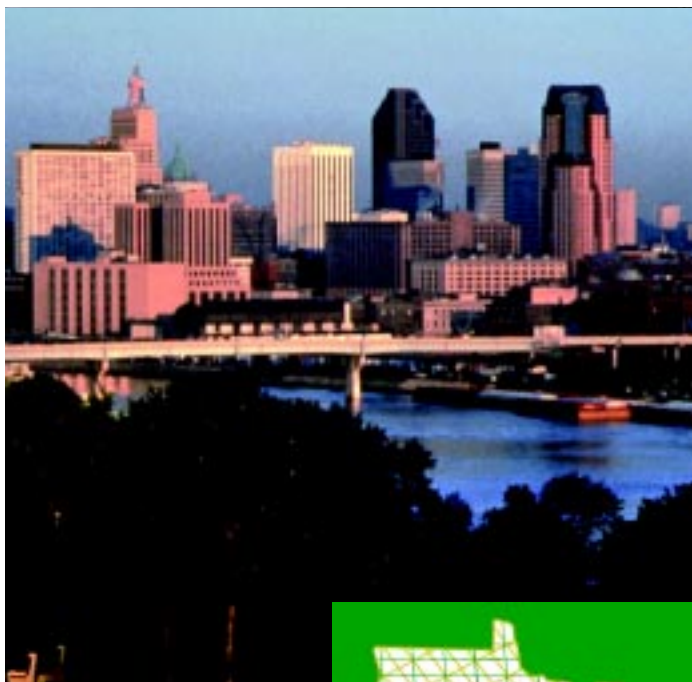


AMERICAN CRYSTALLOGRAPHIC
ASSOCIATION
NEWSLETTER

Number 4

Winter 1999



A central graphic featuring a map of Minnesota with a grid pattern. The text 'MINNESOTA' is written vertically on the left side. The main text reads 'AMERICAN CRYSTALLOGRAPHIC ASSOCIATION' and 'Golden Anniversary Meeting'. Below that, it says 'July 22 - 27, 2000 St. Paul, Minnesota' and 'ACA 2000' at the bottom.



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

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President's column



This is my last column as President and as I write barely six weeks remain until the end of my tenure. I had set two goals at the start; to improve educational opportunities in the field of crystallography and to foster closer ties with South and Central American Crystallographers.. Some progress has been made on both fronts. At the Glasgow IUCr Congress both Bill Duax and I spoke to representatives from Mexico and South America. We informed them of our willingness to have closer relationships and they agreed to hold a caucus. As I understand it they did meet and word came back to Bill that they agree that closer cooperation would be beneficial and how could this be effectuated? Bill drafted a letter to the effect that we would be happy to publish news about the Pan American crystallographic community in the Newsletter. We asked them to appoint a person to act as the official liaison with the Newsletter. We further requested them to form a Special Interest Group (SIG) within ACA with the current 15 ACA members from Central and South America as the core. This group could then plan symposia of interest to their particular needs.

On the education problem, I received three responses in answer to my request in the last ACA Newsletter. Alan Pinkerton wrote that he teaches a four credit course. The first semester covers the theory and some demonstrations (3 credits) and in the second semester (1 credit hour) the students carry out an actual structure solution. John Barnes suggested that the ACA should create a web site specifically designed to provide tutorials on crystallography. Part of the site could include a comprehensive library that would direct the student to review articles, simulation tools, example archives, etc. John indicated that he would be willing to contribute to such a project after he retires and suggests that other emeriti or educators would be willing to participate. Jerry Cohen wrote on 11/3/99 that Northwestern offers an undergraduate course and two graduate courses in crystallography and diffraction with structural techniques offered in one of the graduate courses. He suggested virtual labs in which equipment could be operated on a website. Northwestern will have a website ready in January on powder diffraction at their synchrotron site. Shortly after this communication, I received word that Jerry died suddenly from a heart attack. Jerry was a great practitioner of diffraction methods and a personal friend. I am sure that all his friends and acquaintances will sorely miss him. We wish his family our sincere condolences.

It appears that the use of Internet or WWW in teaching crystallography is the future. Robin Rogers and Krishnamohan Sharma have written a proposal to NSF in which they would provide access to an X-ray diffraction facility to four-year colleges and universities that are without central X-ray facilities through the Internet and video-conferencing facilities. Robin and Krishna would develop the necessary software and hardware necessary to conduct such a program and provide instruction and assistance interactively. Dr. Sharma is currently a post-doc in my laboratory so he would be able to participate fully in the program and use the facilities of my lab as well as those at the University of Alabama. Please feel free to e-mail me with your thoughts on these suggestions.

Let me conclude by stating that it has been a pleasure and an honor serving you as your President and I look forward to many more years of participation in ACA affairs.

Abe Clearfield

Council News

Congratulations to Bill Duax, who was elected to the Executive Committee of the IUCr at the Glasgow meeting. Let me take this opportunity to thank Bill for all the work he does for the ACA as its Executive Officer. We are happy that he will be participating in the work of the IUCr as well.

Did you attend the first ACA meeting held at Pennsylvania State University in 1950? We will be celebrating the 50th anniversary of that meeting at the banquet this July in St. Paul. We encourage all the long-time ACA members to make a special effort to attend the banquet in July, and to let the ACA office know that you will be there, so we can recognize you for 50 years of ACA participation. We welcome contributions — a paragraph or an article — on the history of the ACA for the next Newsletter. Historical photographs would be interesting as well, either to accompany your contribution to the Newsletter or to display at the meeting. For those of you who are curious about the organizations which preceded the ACA, refer to the article by Martin Buerger, “Background and Early History of the American Crystallographic Association” in *Crystallography in North America*, edited by Dan McLachlan, Jr. and Jenny P. Glusker.

The National Institute of Standards and Technology (NIST) is celebrating its centennial anniversary in 2001. We invite contributions to the Newsletter on the history of crystallographic research at NIST.

Perhaps you noticed that the ACA web site has a list of Crystallographic Education Web Sites, which were compiled by Katherine Kantardjieff and myself last summer. If you have additional education sites to suggest, please send them to pett@acs.wooster.edu. Do you have some favorite web sites that you think other crystallographers might like to know about? Take a look at Crystallographic Sites and Crystallographic Resources on the ACA web page. If your favorite isn't listed, please send suggestions to aca@hwi.buffalo.edu.

If you are interested in detailed information about the work of the ACA Council, the SIGs and Standing Committees, you can find it on the ACA web page. The minutes of the ACA Business Meeting (5/24/99), the ACA Council meetings held in May with SIGs and Standing Committees and the May and October Council meetings are available under Updates, Council Reports. If you have any feedback on this new policy of posting the minutes, which was suggested at the Business Meeting by Douglas R. Powell, please send comments to me by e-mail. We hope that posting the minutes will increase communication and encourage more membership participation in the work of our organization.

James H. Stith, the Director of Physics Programs at AIP, described AIP services to member societies at the ACA Council meeting (10/2/99). Under the heading of “Public Information” he described a new Syndicated Science News Service which will sell TV spots on science three times a week. He showed us several examples of Physics Success Stories. These are glossy one-page summaries for legislators that describe successful and significant applications of government-funded research. If you have an idea for a Physics Success Story involving crystallographic research, please send it to Council.

Only a few members returned the Volunteer Survey sheets that were available at the Buffalo meeting. The ACA is notable among scientific societies for the high level of commitment of its membership. We welcome all those who would like to contribute to these efforts. If you want to help but don't know how to begin, take a look at the listing of the SIGs on the ACA web page. I'm sure that the officers would be grateful for any help you could offer.

Doug Ohlendorf, Bill Gleason and Victor Young described their plans for the 50th ACA meeting in July, 2000. Ohlendorf is organizing two workshops: “How to Make Technical Oral Presentations on Crystallography” and “SHELX for Twins and Macromolecules.” The *Transactions* Symposium will be “Using Crystallography to Understand Enzyme Mechanisms.” This will be an excellent program in a great setting, the River Centre of St. Paul.

This is my last column as Secretary of the ACA. I've enjoyed working with the other Council members and participating in an organization that has contributed greatly to my scientific development.

Virginia Pett

Reminder

Y2K Dues are Due

Don't forget your favorite ACA funds

Jerome B. Cohen (1932-1999)

Jerome (Jerry) B. Cohen, whose expertise was in materials science, spearheaded a transformation of the engineering school at Northwestern University, revamping the curriculum, recruiting top-flight faculty members and presiding over an ambitious building plan. After 13 years as dean of the Robert R. McCormick School of Engineering and Applied Science, he was looking forward to semi-retirement, having given up his administrative duties in September to return to the classroom. He passed away in early November of an apparent heart attack after a morning swim. He was 67.

A graduate of the Massachusetts Institute of Technology, he came to Northwestern in 1959 as an assistant professor of materials science and engineering. He became dean in 1986. It was his innovations in undergraduate course work for which he was most noted, transforming the methodology of teaching engineering at the college level. He also encouraged engineering students to participate in joint studies in medicine, music, law, journalism, education and management, believing they could use their talents in applying math and logic to become leaders in any field.

A metallurgist with a passion for race cars, Jerry was highly regarded with a long list of awards and honors to his name, including a Fulbright scholarship in the late 1950s. Even as dean, he continued to carry out important research in the use of X-ray diffraction in understanding the nature of materials. He performed work at Argonne National Laboratory under funding from Dow Chemical and the DuPont Corp. and has several patents attributed to him, including one for a method of making beryllium alloy.

He is survived by his wife, Lois; a daughter, Elissa Halpern; a son, Andrew; and four grandchildren.

Megan O'Matz

Helen Berman wins Biophysical Society Distinguished Service Award

Helen Berman (Rutgers), is the year 2000 recipient of the Biophysical Society's Distinguished Service Award. The award, established by the Biophysical Society in 1991, honors not only service in the field of biophysics, but also contributions beyond achievements in research. It will be presented at the Society's 2000 Annual Meeting, February 12-16, 2000 in New Orleans, LA.

Helen is a member of the Faculty of Arts and Sciences-Rutgers New Brunswick. She and her research team were the first scientists to produce detailed pictures of the triple helix of collagen, the most common protein in the human body. She also headed the team that established the Nucleic Acid Database, which provides information through the Internet on the three-dimensional structures of nucleic acids. She joined Rutgers in 1989 and teaches courses in biophysical chemistry and X-ray crystallography. Under Helen's direction, Rutgers has become the lead institution managing the new PDB.

"Helen Berman has a long history of outstanding scientific contributions to deciphering the structures of critical biological molecules, initially and notably with DNA and its components," said Dr. Jonathan King, president of the Biophysical Society. "Her efforts have been marked by extraordinary service to the broader scientific community. She has now embarked on a new stage, reorganizing and raising to a higher level of accessibility and creativity the Protein Data Base, an international resource that provides tools for thousands of scientific workers."

Joseph Blumberg

Abe Clearfield Named Sigma Xi 1999 TAMU Distinguished Scientist

Abe Clearfield, who leads Texas A&M in the area of materials science, received his B.A. in Chemistry and M.A. in Physical Chemistry (Kinetics) from Temple University and his Ph.D. in Inorganic Chemistry Crystallography from Rutgers University. He has had a varied career in government, industry and academia. One colleague writes, "In my opinion, Professor Abraham Clearfield represents the highest ideals of science at Texas A&M." Clearfield has published hundreds of articles and papers including the classic paper in Chemical Reviews on "The Role of Ion Exchange in Solid State Chemistry." The paper showed the connection between facile inorganic ion exchangers, super-ion conductivity and the use of ion exchange methods in solid state synthesis. In 1985, he initiated the highly successful Materials Research Program, a program that now has external funding exceeding ten million dollars annually. With a expertise in nuclear waste containment that is unparalleled at Texas A&M, Clearfield recently teamed with scientists at the Institute for Problems of Sorption and Endoecology in Kiev, Ukraine to help with the environmental problems created by the Chernobyl Nuclear Explosion. As a result of these efforts, he has been nominated as a foreign member of the Ukraine National Academy.

Sigma Xi Press Release

Queen's Principal Appoints Suzanne Fortier New Vice Principal (Academic)

Queen's University (Ontario, Canada) has announced the appointment of Suzanne Fortier as Vice-Principal (Academic), effective July 1, 2000. She is currently completing her 5th year as Vice-Principal (Research). The announcement stated that "Suzanne's broad knowledge of Queen's, her outstanding reputation nationally and internationally, and her unwavering dedication to excellence in teaching and research will be important assets in her new role as VP Academic". A crystallographer by training, she is currently a professor of chemistry and also holds a professorship in the Department of Computing and Information Science.

Crystallographers Named as Fellows by the Biophysical Society

The Biophysical Society has announced the Society Fellows for the year 2000. This first class of Fellows consists of 39 distinguished Society members who have contributed to the highest level of the science of biophysics and includes a number of crystallographers.

Donald L. D. Caspar (Florida State U) for his pioneering research in structural biology including determination of the first viral structures by X-ray diffraction, and for his insightful work on viruses and structures of crystals.

David Eisenberg for his unique contributions to the understanding of protein structure and stability using X-ray crystallography and computational modelling, and for relating structure to function by biochemical and genetic methods.

Barry Honig for his many seminal contributions in biophysics including quantum chemistry, biophysics of color vision, protein folding, electrostatics of proteins in DNA and protein structure prediction and bioinformatics.

Hugh E. Huxley (Brandeis) for establishing the structural basis for muscle contraction using X-ray diffraction and electron microscopy.

Frederic M. Richards (Yale) for seminal contributions to methods of protein structure determination, for a long history of contributions to protein structures, and for deep insights into the forces of organization, packing, and geometries in proteins.

Michael G. Rossmann (Purdue) for his fundamental contributions towards the determination of the 3-D structure of viruses accomplished over many years by his methodical and creative development of mathematical procedures, unique biochemical and crystallographic techniques, and for identifying the Rossman fold.

Robert M. Stroud (UC San Francisco) for his leadership for many years in shaping the field of X-ray structural studies of structure-function relationships in macromolecules and for his mentoring an extraordinarily successful group of graduate students and postdoctoral fellows.

Biophysical Society Press Release

Call for Nominations for the USNCCr

The USNCCr will be electing four new regular members in 2000 to serve for the three year period 2001-2003. Members must be currently active in some area of crystallography and must be a permanent resident of the US. If you would like to nominate someone, including yourself, to serve on the Committee, please contact one of the following USNCCr members:

Cynthia Stauffacher, Chair	cyndy@gauguin.bio.purdue.edu
Peter Buseck	pbuseck@asu.edu
Bing Jap	jap@rhoda.lbl.gov
Ian Robinson	ikr@uiuc.edu

Protein Data Bank Update

The Research Collaboratory for Structural Bioinformatics (RCSB) began its second year of managing the Protein Data Bank on October 1, 1999. It was at this time last year that the RCSB began a transition so successful that it ended on July 1, 1999 — a full three months ahead of schedule.

During this past year the PDB released ADIT, the AutoDep Input Tool, which is used for structure deposition at <http://pdb.rutgers.edu/adit/>. A specialized version of ADIT is used by the PDB to process the deposited data for inclusion in the archive, and has been used for over 2,600 structures. Approximately 500 of these were unreleased structures inherited by the RCSB at the time of the PDB transition in various stages of processing. Another 456 of these structures were released as “Layer 1” entries — meaning unannotated and unprocessed — and brought them to “Layer 2” status for release in the near future. The PDB fully processes files at the time of deposition with an average turnaround time of less than ten days.

The PDB can be queried at <http://www.rcsb.org/pdb/> using SearchLite and SearchFields. SearchLite provides a text box for simple keyword searching, while SearchFields allows the combination of fields to search specific items of data that are important in the representation of the structure and the experiment. The resulting structures can be examined individually or as a set. The PDB can also be searched for the status of unreleased structures. The primary PDB site receives a query at the rate of one query per minute, twenty-four hours a day, seven days per week.

Since the completion of the PDB transition on July 1, RCSB PDB mirror sites have been established at the National University of Singapore, Singapore and Osaka University, Japan. RCSB PDB mirrors will be available at the Cambridge Crystallographic Data Center, UK and at the Universidad Federal de Minas Gerais, Brazil in the very near future. The full list of RCSB PDB mirror sites is available at <http://www.rcsb.org/pdb/mirrors.html>. In addition, new applications and query enhancement are now being staged for public testing and comment at a beta test site (<http://beta.rcsb.org/pdb/>) before they are moved to the production sites. All PDB users are invited to try out the new applications.

The PDB plans to focus on the Data Uniformity Project in the coming year. The content and format of the PDB entries have changed over the past twenty-five years. In order to improve the query capabilities of the PDB search engines and those of other database resources, these data need to be made uniform. A variety of tools and procedures have been put in place to facilitate the process. PDB users will begin to see the impact of these efforts in the coming months.

Current news and information about the PDB is available at <http://www.rcsb.org/>. Questions and comments about the RCSB PDB project should be sent to info@rcsb.org.

Christine Zardecki

**AMERICAN CRYSTALLOGRAPHIC ASSOCIATION, INC.
BALANCE SHEET
JUNE 30, 1999 AND 1998**

	CURRENT FUNDS		TOTAL	
	Unrestricted	Restricted*	All Funds	
			1999	1998
ASSETS				
Current Assets:				
Cash	90,367	318,758	90,357	315,587
Investments	516,159			532,600
Inventory	100		100	100
Total Current Assets	606,626	318,758	925,384	848,287
Fixed Assets:				
Computer	15,969		15,969	15,969
Office Equipment	3,194		3,194	
Accumulated Depreciation	-19,163		<19,163>	-19,163
Total Fixed Assets	0	0	0	0
TOTAL ASSETS	606,626	318,758	925,384	848,287
LIABILITIES & FUND BALANCE				
Liabilities:				
Income Tax Payable	0		0	0
Deferred Dues Income	69,242		69,242	71,233
Deferred Meeting Income	0		0	3,652
Total Liabilities	69,242		69,242	74,885
Fund Balance:				
Unrestricted	537,384		527,384	496,817
Restricted	318,758		318,758	276,585
Total Fund Balance	537,384	318,758	856,142	773,402
TOTAL LIABILITIES & FUND BALANCE	606,626	318,758	925,384	848,287

* Current Balances in individual restricted funds - as of June 30, 1999

Patterson Award	33,937
Fankuchen Award	64,791
Buerger Award	31,838
Pauling Award	29,230
Etter Award	76,128
Supper Fund	10,374
Wood Fund	45,453
Warren Award	<u>27,007</u>
	318,758

A more detailed report on the ACA finances may be obtained by sending a written request to the ACA office in Buffalo, PO Box 96, Ellicott Station, Buffalo, NY 14205-0096

ACA CORPORATE MEMBERS

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

ATPS Inc.
atpsinc@aol.com

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Hannover, Germany

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blake4xray@worldnet.att.net

Bruker AXS Inc.
www.bruker-axs.com

Charles Supper Company, Inc.
www.supper.com

Compaq Computer Corp.
www.compaq.com

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

Crystal Logic Inc.
www.xtallogic.com

Cyberlab
www.cyber-lab.com

Fuji Medical Systems USA, Inc.
www.fujimed.com

Hampton Research
www.hamptonresearch.com

HHMI/Sigler Lab
www.hhmi.org

J Schneider Elektrotechnik GmbH
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jstoll@lepel.com

Microsource
www.bede.com/micro.html

Molecular Structure Corp.
www.msc.com

Nonius Company
www.nonius.com

Osmic, Inc.
www.osmic.com

Oxford Instruments
www.oxfordinstruments.com

Protein Data Bank
www.rcsb.org/pdb

Protein Solutions, Inc.
www.protein-solutions.com

UOV/Biblioteca Universitaria
Oviedo, Spain

X-Ray Research GmbH
www.marresearch.com

Perspectives in Structural Biology A volume in honour of G.N. Ramachandran, Eds. M. Vijayan, N. Yathindra, and A. S. Kolaskar (ISBN: 81 7371 254 9; Paperback; 180 x 240mm; 764pp) Published by Universities Press in collaboration with the Indian Academy of Sciences.

Prof. G. N. Ramachandran, FRS, has been among the foremost biophysicists and structural biologists of our times and the most outstanding scientist to have worked in independent India. His contributions pertaining to collagen, methods of structural analysis, computer modelling and conformational analysis, and three-dimensional image reconstruction have had a global impact. This volume in his honor consists of articles at the cutting edge of structural biology contributed by leading scientists, including two Nobel laureates. It is intended to be a window to modern structural biology and a showcase to the Indian effort in this area.

Contributors: M.F. Perutz, M. Vijayan, J. Kuriyan, K. Drickamer, D.M. Salunke, A. Imberty, J.L. Whittingham, N.W. Isaacs, V. Pattabhi, D. Pietrobon, J.K. Dattagupta, W.G.J. Hol, F. Parak, M.R.N. Murthy, T.P. Singh, K.R.K. Easwaran, Ch. Betzel, E. Benedetti, K.K. Kannan, A. Saran, D. Moras, M. Sundaralingam, B.W. Matthews, E. Westhof, V. Sasisekharan, N. Yathindra, H.M. Berman, R.V. Hosur, C. Ramakrishnan, M. Maiti, T.L. Blundell, N. Gautham, R.L. Jernigan, M. Bansal, J. Janin, H.A. Hauptman, P.L. Privalov, S. Parthasarathy, R. Varadarajan, E.N. Baker, H.A. Scheraga, M.G. Rossmann, J.B. Udgaonkar, J.L. Carrascosa, R.L. Baldwin, S. Vishveshwara, P. Balaram, J.M. Claverie, P.K. Ponnuswamy, U. Heinemann, L.N. Johnson, N. Niimura, N. Srinivasan, G. Govil.

Madhu Reddy (upilco@hd2.dot.net.in)

ACA Election Results

Vice-President
Secretary

William Stallings
Lee Brammer

New Standing Committee Members

Apparatus & Standards
Data & Computing

Victor G. Young, Jr
John C. Huffman

Continuing Education
Publications

Bryan Craven
Frank Rotella

Special Interest Groups

Amorphous Materials
Chair-elect

Priya Vashishta

Service Crystallography
Chair-elect

Lee Daniels

Biological Macromolecule
Chair-elect
Secretary

P. Lynn Howell
Jack Sack

Small Angle Scattering
Chair-elect
Secretary / Treasurer

Andrew Allen
Jinkui Zhao

General Interest
Chair-elect

David J. Duchamp

Small Molecule
Chair-elect
Secretary / Treasurer

Joe Reibenspies
Curt Haltiwanger

Materials Science
Chair-elect

Scott Misture

Synchrotron Radiation
Chair-elect

Dick Harlow

Neutron Scattering
Chair-elect

Bryan Chakoumakos

Young Scientists
Chair-elect

Matthew Vetting

The proposed changes to the Bylaws - Rule III - Committees - were accepted by the membership.

Rule III Section 3 - Number of members in each committee will be 4 members each serving a 4 year term starting 1/1/2001

Rule III Section 6 - Names (and number) of Committees. There will be three named:

Continuing Education; Data, Standards and Computing; and Communications

New ACA Vice President - Bill Stallings



I first met Bill Stallings, in 1987 when I was responsible for hiring a protein crystallographer to fill a position at Monsanto Corporate Research. While conducting the search, Bill Stallings' name kept coming to me, with the highest possible recommendations. I had known of Bill's work, particularly that on superoxide dismutase, but had not known him personally. This work, done in collaboration with Martha Ludwig at the Univ. of Michigan, led to our current understanding of the structure-function relationship of iron and manganese superoxide dismutases. Bill went to Michigan in 1980 from the Inst. of Cancer Res. where he had been an NIH Postdoctoral Fellow and Research Assoc., working with Jenny Glusker. In Jenny's lab, Bill worked on the structure determination of compounds with antitumor properties. This came on the heels of his PhD work with Jerry Donohue at the Univ. of Pennsylvania, where among others, he determined the structure of biotin.

Bill joined Monsanto in 1988, where I had the privilege to work with him. I have known him since, not only as a colleague but also, as a friend. His scientific accomplishments at Monsanto are numerous, of which his work on the structures of EPSP synthase, HIV protease and cyclooxygenase-2 are but a few. His work on the structure of EPSP synthase showed a novel fold and molecular symmetry and allowed Monsanto's scientists to evaluate many of their ideas for the design of new herbicides. Bill also played a critical role in the design of Searle's (Monsanto's Pharma Sector) HIV-1 protease inhibitors that made it to the clinic.

Although I left Monsanto in 1990, my scientific interest and that of Bill's met again in 1996 when we both realized that we had determined the same structure, that of human cytomegalovirus protease, a serine protease that is essential for that virus lifecycle, and discovered yet another novel fold and catalytic triad. Instead of trying to beat each other to press, we agreed to publish back-to-back. Although much of Bill's other work is shrouded in company secrets, his group has published very exciting work on the structural basis of cyclooxygenase-2 ligand selectivity. Because of his many accomplishments, Bill was promoted very quickly at Monsanto/Searle where he is currently responsible for all structural and computational chemistry.

In addition to his considerable research accomplishments, Bill has also been a very active member of the ACA. He was Program Chair of the 1997 ACA in St. Louis, and is currently a co-editor of *Acta Cryst.* It has been a joy for me to have had the opportunity to work with Bill. This joy is shared by everyone I know who has interacted with him. The ACA is fortunate to have him as its new Vice President. Please join me in wishing Bill the best.

Sherin Abdul-Meguid.

New ACA Secretary - Lee Brammer



Lee is a native of Barnsley, England and received his undergraduate and graduate degrees from the Univ. of Bristol in the U.K. He received a B. Sc. (Hons) degree in 1983 and his PhD degree in inorganic chemistry in 1987 under the direction of Professor A. Guy Orpen. He moved to the USA for a 20-month post-doctoral fellowship with Ed Stevens at the Univ. of New Orleans and then spent two years with Tom Koetzle at the Brookhaven National Lab.. He joined the Univ. of Missouri- St. Louis as an Assistant Professor of inorganic chemistry in 1990 and was promoted to the rank of Associate Professor in 1996 at the age of 33!

Lee has received national and international awards for his research in crystallography including a NATO Postdoctoral Fellowship (1987-89) and the S. S. Sidhu Award of the Pittsburgh Diffraction Society in 1990. He has been very active in ACA and IUCr activities as well as in the ACS. Lee has served on a number of committees of the ACA and was the local chair of the very successful St. Louis ACA meeting in 1997. He was the Chair of the Pauling Prize Committee in 1994 and 1995, and Chair of the 1999 Patterson Award Committee. He was a member of the Data and Computing Committee during 1996-98. Lee has served as a member of the IUCr commission on journals since 1996 and a member of IUCr Commission on Structural Chemistry since 1999. Lee has been a Co-Editor of the *Acta Cryst C* since 1996.

Since joining the University of Missouri- St. Louis, Lee has developed a highly productive research program. Lee's research interests are focussed on the role of transition metals in both crystalline-phase and solution-phase supramolecular chemistry, on the investigation and application of hydrogen bonding in organometallic chemistry, electron density studies of transition metal-hydrogen interactions and on the structure and bonding questions in transition metal organometallic chemistry. Lee has been recognized as an authority on inter and intra-molecular hydrogen bonding due to his pioneering contributions in the field. He has received external funding for his research at UM- St. Louis, and also for the organization of international symposia. Lee also teaches graduate level crystallography which is a very popular course in the department.

The ACA is very fortunate to have Lee as its new Secretary and I have enjoyed working with him for the past nine years. We share diffractometers in the X-ray laboratory and interesting discussions on crystallography in the office corridors and at lunchtime seminars. Literally, crystallography is a major part of Lee's life since he is also married to a crystallographer, Dr. Louise Cunane. We can look forward to a very productive term under Lee's tenure as Secretary.

Nigam Rath

1999 ACA Summer Course in X-ray Crystallography at the University of Georgia, July 12 - 24

The 8th annual ACA Summer Course in Crystallography was held at the Georgia Center for Continuing Education on the Univ. of Georgia campus from July 12 - 24, 1999. The 48 students came primarily from 21 states in the US with 2 from Canada. Our most far-flung student, Mahaela Maria Pop, came on her first trip to the US from Babes-Bolyai University in Cluj-Napoca, Romania.

Mornings were devoted to lectures about the theory and practice of crystallography and X-ray diffraction. In the afternoons, students gained hands-on experience with crystal growth, mounting and data collection techniques involved in both small molecule and macromolecular crystallography. Lectures and/or discussions on advanced or special topics were held in the evenings.

During the 8 days of the small molecule portion of the course, students had the opportunity to work on numerous structural problems using previously measured data. Some students brought their own crystals for data collection. In all, about 14 new data sets were measured and analyzed successfully. At least one structure determined during the Summer Course is currently in press.



*Small Molecule
Students and Teachers*

There were 24 course lecturers and laboratory tutors contributing to the success of this year's Summer Course. Lecturers for the small molecule and fundamentals portion of the course were: Bryan M. Craven (Indiana University of Pennsylvania), Steve Geib (University of Pittsburgh), Jenny Glusker (Fox Chase Cancer Institute), Herbert Hauptman (Hauptman-Woodward Institute), Gary Newton (UGA), Ward Robinson (Bruker AXS and Canterbury University, New Zealand), John P. Rose (UGA) and Robert A. Sparks (Bruker AXS consultant). Macromolecular lecturers were: Paul Adams (HHMI/ Yale U.), Chun-Jung Chen (UGA), Robert Cudney (Hampton Research), Jeffrey Habel (University of Toledo), Leigh Ann Lipscomb (UGA), Zhi-Jie Liu (UGA), Cory Momany (UGA), John P. Rose (UGA), Robert Sweet (Brookhaven National Laboratory), Thomas Terwilliger (Los Alamos National Laboratory), Bi-Cheng Wang (UGA), Chia-Kuei Wu (UGA).

Several lecturers also participated in the laboratory sessions. Principal tutors and assistants in the small molecule laboratory sessions were: BRUKER - Ward Robinson and Steve Geib; MOLECULAR STRUCTURES CORP. - Kris Tesh (MSC) and John P. Rose; NONIUS - Anita Coetzee (Nonius, Inc., Delft, The Netherlands), Dan Frankel (Nonius, Inc. USA) and Don Woo Lee (Georgia State University).



*Macromolecular
Students and
Teachers*

For the first time all three laboratories had area detectors available for data collection. In previous years the students had to wait for long data sets to be completed before new samples could be mounted. As a result, this year, there were fewer time constraints and the laboratory sessions were much more relaxed and productive.

Macromolecular laboratory and workshop sessions were directed by Paul Adams, Chun-Jung Chen, Robert Cudney, Stephen Foundling (Bruker AXS), Jeffrey Habel, Zhi-Jie Liu, John P. Rose, Robert Sweet, Thomas Terwilliger and Chia-Kuei Wu

The ACA Summer Course is again very grateful for the generous support of the ACA, The University of Georgia, Bruker AXS, Hampton Research, Molecular Structures Corporation and Nonius, Inc. The 9th annual ACA Summer Course in X-ray Crystallography is scheduled for July 7-19, 2000 at the University of Georgia. Check web page <http://bcl15.bmb.uga.edu/aca2k.html> for the latest information..

Gary Newton

The 18th General Assembly of the International Union of Crystallography, Glasgow, Scotland, 4-13 August 1999

The 18th General Assembly was held in conjunction with the triennial Congress of the Union, held this year from August 4 – 13, 1999 in Glasgow Scotland. The scientific sessions and commercial exhibits were held in the Scottish Exhibition and Conference Center in Glasgow and delegates were housed in hotels and dormitories throughout the city. The Congress drew over 2200 attendees from 53 different countries. More than half of the attendees came from Europe and Scandinavia (~500 from the UK, ~200 from Germany and ~120 from France). North America accounted for ~450 attendees (mostly from the US) with Asia bringing over 300 (~230 from Japan and ~50 each from Australia and Russia). The remainder of the delegates came from Central and South America (~30), the Middle East (~25) and Africa (~15). Over 2500 abstracts were received, covering all aspects of crystallography and its applications, and included in the Abstract Book. For the first time attendees were also presented with a CD which contained the abstracts and other pertinent crystallographic information.

The US delegates to the Glasgow Assembly were Judith L. Flippen-Anderson (Naval Research Laboratory), Abraham Clearfield (Texas A & M), William Duax (Hauptman-Woodward Research Institute), Marvin Hackert (University of Texas at Austin), and James Kaduk (BP/Amoco). All delegates were present for all sessions of the General Assembly. The alternates, whose services were not required during the actual Assembly meetings, were Connie Chidester (Pharmacia/Upjohn), Jane Griffin (Hauptman-Woodward Research Institute), Jon Clardy (Cornell University), Robert Bryan (University of Virginia) and Howard Einspahr (Bristol Meyers Squibb). With exception of William Duax, Robert Bryan (both former chairs of the USNCCR) and Jon Clardy, all of the delegates and alternates are current members of the USNCCR.



In Scotland: Backrow - Howard Einspahr, Connie Chidester, Jim Kaduk, Jane Griffin, Robert Bryan. Front row - Abe Clearfield, Judy Flippen-Anderson, Bill Duax and Marv Hackert

The 18th General Assembly met in three sessions chaired by IUCr president Ted Baker (New Zealand), with the Executive Committee of the Union and 77 delegates representing 37 countries being present. There were no delegates from Bulgaria, Serbia or the Ukraine and due to a confusion of paperwork the Venezuelan delegate, although present, could not vote. (A copy of the Agenda for the General Assembly, a list of the Executive Committee members for the period 1996-99, and a complete list of delegates to the Assembly can be found at the IUCR website www.iucr.ac.uk).

The first session of the Assembly in Beijing (1993) and in Seattle (1996) began with consideration of applications for membership in the IUCr from a number of new adhering bodies, which reflected the political changes that have taken place in Europe and Asia. There were no such applications in Glasgow, however, two countries submitted requests for changes in their Adhering Bodies. Both requests were approved. The Dutch Association for Crystallography will replace the Royal Dutch Academy as the Adhering Body for the Netherlands, however, the Academy will continue to pay the membership fees in Category II. The British Crystallographic Society will replace the Royal Society as the Adhering Body for the UK and it will also pay the subscription fee in Category V. The report of the Executive Committee of the Union was accepted, as was the Financial Report. The IUCr remains in generally good health with an increase in fund accounts of 21% (disregarding exchange-rate fluctuations) over the triennium. No dues increase was requested (the last increase was in 1993).

The reports of the various Commissions of the Union were presented and accepted, as were those of the representatives on Regional and Scientific Associates of the IUCr (Philip Coppens reported on the ACA as a regional associate) and of IUCr representatives on other scientific bodies, principally ICSU and its various committees. The first formal report of the Database Committee, which was established in Seattle in 1993, was presented and accepted. A representative from each of the Committees and Commissions had met with the members of the Executive Committee before the start of the General Assembly and the President reported that most of the Commissions seem to be functioning effectively in pursuit of their chartered objectives.

For the first time in its history there were two candidates for the office of President of the IUCr, Henk Schenk of the Netherlands and Hartmut Fuess from Germany. Both candidates made short presentations at the beginning of the second session of the General Assembly. The Delegates then confirmed Jerusalem, Israel as the location for the 19th IUCr Congress and General Assembly in 2002. They then listened to and watched presentations from Florence, Italy and Nagoya, Japan both of which had been proposed as potential sites for the 20th Congress in 2005. At its third session the Assembly voted in favor of Florence. At that same session the delegates voted to approve the slate of Commission Members and Chairs offered by the Executive Committee. The following U.S. Crystallographers were among those nominated by the IUCr Executive Committee, and elected to membership in IUCr Commissions for the 2000-2002 triennium: Viet Elster (*Aperiodic Crystals*), Eddie Arnold and Janet Smith

(*Biological Macromolecules*), A. Bansil and J. Spence (*Charge, Spin and Momentum Densities*), D. Bliss (*Crystal Growth and Characterization of Materials*), John Westbrook and P. White (*Crystallographic Computing*), Sidney Abrahams (*Chair, Crystallographic Nomenclature*), Carol Brock and Margaret Kastner (*Crystallographic Teaching*), Doug Dorset (*Chair*) and J. Spence (*Electron Diffraction*), Sol Gruner, R. Hemley and John Parise (*High Pressure*), Jim Jorgensen and Brian Toby (*Neutron Diffraction*), Robert VonDreele (*Powder Diffraction*), John Barnes (*Chair*) and P. Thiyagarajan (*Small-angle Scattering*), Judy Flippen-Anderson (*Chair*) and Lee Brammer (*Structural Chemistry*), Sol Gruner and Ian Robinson (*Synchrotron Radiation*) and J. Penner-Hahn (*Chair*) and S. Heald (*XAFS*). Gary Gilliland was confirmed as the representative to the ICSU Committee on Data for Science and Technology (CODATA) and Helen Berman was reconfirmed as the Chair of the ad hoc Data Base Committee which the Executive Committee had created in Seattle (1996) to replace the Data Base Commission.



Your reporter spent the mid-meeting day off enjoying the beautiful sites of Edinburgh

One of the IUCr's main functions is the publication of most of the leading journals in crystallography: *Acta Crystallographica*, Sections A-D, the *Journal of Applied Crystallography* and the *Journal of Synchrotron Radiation*. Jenny Glusker (US) was reconfirmed as the Editor of *Acta Crystallographica Section D* that concentrates on biological macromolecules. In addition, there are US Co-editors serving on all of the IUCr Journals. The Union also publishes books and a seven-volume set of International Tables covering the various areas of crystallography. Two of the seven are edited by American crystallographers: *Volume C. Mathematical, Physical and Chemical Tables*, edited by Ted Prince and *Volume F Macromolecular Crystallography*, edited by Michael Rossmann and Eddie Arnold. Finally, the Union publishes a *Newsletter* that is produced 4 times a year and sent,

free of charge, to all crystallographers listed in *the World Directory of Crystallographers*. US crystallographer William Duax was reconfirmed as the Editor of the *IUCr Newsletter*. Concerned with increasing costs of producing and distributing hard copy publications, as well as with the decrease in subscriptions, the Union is moving strongly towards electronic publication including CD ROM versions of journals and tables. Progress in this endeavor is good and was reported on during the General Assembly meetings.

Elections for the officers of the Union were also held during the third session of the General Assembly. The balloting for President of the Union resulted in the election of Henk Schenk (Netherlands). The second candidate, Hartmut Fuess (Germany) will remain on the Executive Committee to complete the six-year term as an Ordinary Member for which he was elected in Seattle. M. Tanaka (Japan) was confirmed as the Union Vice-President and Sine Larson (Denmark) was confirmed for a second term as General Secretary/Treasurer. With the election of Henk Schenk, Ted Baker (New Zealand) automatically assumed the office of Past-President. The Executive Committee had presented a slate of five candidates for the three six year vacancies for Ordinary Members of the Executive Committee. In addition, Judith Howard (UK) was nominated by petition bringing the total list of candidates to six. A majority of the votes cast are necessary for election. Bill Duax (US) and Maria Carrondo (Portugal) were elected in the first round of balloting. If no candidate receives a majority of the ballots cast then the candidate receiving the lowest number of votes is dropped and the balloting is repeated. It took three more rounds of balloting before Z. Zhang (Peoples Republic of China) was elected to the Executive Committee. The election of M. Tanaka as Vice-President created a three-year vacancy on the Executive Committee, which necessitated a second full round of balloting. The Executive Committee had originally proposed a slate of six candidates for this position, which was raised to seven by the addition of the nomination from the floor. However, the elections of Duax, Carrondo, and Zhang reduced the number to four. Two rounds of balloting were needed to elect Jan Boeyens (South Africa) to fill this vacancy. He had been elected to a three-year term, under similar circumstances, in Seattle. At the close of the Congress two US crystallographers, Phillip Coppens and Michael Hart, completed their service on the Executive Committee. A second North American candidate for the Executive Committee, Suzanne Fortier (Canada) was also among the nominees for Ordinary Member.

Following the elections a discussion ensued regarding the overall length of the Congress currently set at 10 days of scientific sessions. After approximately one half hour of discussion the Chair of the US Delegation made a motion to shorten the meeting to seven days of scientific sessions to take effect with the 2005 meeting. The motion was seconded by the Canadian Delegation, no further discussion followed, and the motion carried unanimously. The President then adjourned the third session of General Assembly and since all business had been conducted it was not necessary to hold the scheduled fourth session.

General Observations on the Future:

The IUCr is currently in good health, both scientifically and financially. The new Executive, under President Henk Schenk is well qualified to maintain a progressive leadership role. The new US member of the Executive, Bill Duax, brings a wealth of experience to the Committee having served as President and Executive Officer of the ACA, Chair of the USNCCr, and Program Chair for the 17th Congress and General Assembly of the IUCr in Seattle in 1996. Plans are well underway for the next General Assembly in Jerusalem in 2002 and we expect to see an expansion of the role played by electronic presentations.

As with many other scientific journals the number of subscriptions to hard copy IUCr publications has been declining due to increasing costs and decreasing availability of storage space. To counteract this trend the Union has been moving strongly towards electronic publication of its journals and appears well poised to accomplish this transition. To remain competitive in an arena that has seen a number of new journals inaugurated in the past few years the Union hired a Promotions Representative in 1998. Since then, a campaign to market the IUCr journals and services more aggressively to the crystallographic community as well as to structural science communities in biology, chemistry, materials science and physics has begun.

If these efforts are successful it should be possible for the Union to continue to provide financial support for student travel and satellite meetings occurring in the interim between Congresses without the need for an increase in dues in the near future.

Judy Flippen-Anderson, Chair US Delegation

Young Scientist Travel Awards for IUCR 18 in Glasgow

Due to the financial success of the 17th IUCr Congress in Seattle the USNCCr was able to offer travel grants for attendance at the 18th Congress. Other US institutions, NASA, the International Centre for Diffraction Data (ICDD) and the American Crystallographic Association (ACA) also made funds available for this purpose. The Research and Travel Grants subcommittee of the USNCCr, (Jane Griffin (Chair), Mike Hart, Lee Brammer, and Howard Einspahr) administered the program in concert with a group from NASA chaired by Eddie Snell. Graduate students and PhDs within three years of graduation, living and working in the US, were eligible for the travel awards. It was also necessary to be presenting a paper (poster or oral) at the meeting. A total of 49,360 dollars were available (USNCCr – 17,000, NASA – 21,000, ICDD – 10,000 and ACA 1,360) for distribution. This amount made it possible to fund 43 awards with the average being 1,100 dollars (smallest award was 800 and the largest was 1500). Most of the awards were made by pre-paying registration and dorm fees. I am extremely pleased by this program and feel that it is a clear indication of the continuing strength of crystallographic research in the United States. Please keep reading for comments sent to us by some of our travel awardees.

Jane Griffin

Life in the Trenches - Reports from Travel Award Grantees

I would like to thank you and the entire committee for the generous support that you provided for my attendance at the International Union of Crystallography meeting in Glasgow.

I was able to present my research, and enjoyed discussing it with others who offered new insights. I was also able to learn more about many other areas. It was a very worthwhile experience. I would like to say that after sitting in

the membrane session, I was able to rush home and immediately crystallize the membrane protein with which I am working, but I can't. But I was able to get some good ideas to try and new enthusiasm.

Monica Niederhut, Indiana University School of Medicine, Indianapolis, IN

This is my reply to the request for a report on the effect the IUCr meeting has had on my research. I think there are several important points:

1. It gave me a chance to present a poster on our research, and talk about various aspects of our research with people who have more experience and/or a different way of looking at things.

2. Getting an impression of what other people are doing in the methods field. Methods is a relatively small discipline and this is one of the few occasions where most of the people in this field get together. And listening to a talk can give you a more direct idea of the ideas behind the programs and algorithms than just reading the article.

3. Personal development. Even when you go to lectures that are not directly related to your field, you gain a broader understanding of crystallography as a whole. And often you will find an idea that might be applicable to your specific problem.

Jaco van der Plas - Purdue Univ, West Lafayette, IN

Firstly I should thank the various organizations for providing funds to help me travel to and attend the IUCr Congress in Glasgow, Scotland. It was very exciting to attend such a large meeting and see the importance crystallography has in cutting edge scientific research in a tremendous number of areas.

My personal highlight was the presentation by Hugo Rietveld, particularly because my research involves Rietveld analyses on powder samples.

For a young researcher I had the opportunity to present my work in a poster session and could discuss the more challenging aspects in detail with a number of people. Also, importantly, I have been able to make new contacts and meet possible future collaborative research partners.

The plenary lectures were set at levels which were understandable by non-specialists, and covered a broad range of science. The scientific programme proved to be enjoyable, although very hectic rushing between overlapping sessions and presentations. Presentations I attended varied from techniques which could have a revolutionary impact (holography), to future

commercial applications stemming from an understanding of the crystallography (Li-ion battery materials).

For me the primary interest lay in the study of powder materials, and how software and instrument/equipment developments are beginning to impact many problems which were previously unsolvable. It was refreshing though to not only hear the progress made, but also to see the complex issues that still must be understood and overcome.

I came away from this conference with many new helpful ideas and a better understanding in a number of areas. I hope to apply this knowledge to the direct benefit of my research now and in the future.

Brian Mitchell, IPNS, Argonne, IL

It was a marvelous opportunity to attend the IUCr meeting in Glasgow this year. This was the first IUCr meeting that I have been able to attend and I was very much impressed by the conference. There was a great variety of topics, a high standard of research on display and ample opportunity to interact with a wide variety of researchers from across the globe. I hope that this will be the first of many IUCr conferences in which NASA representatives and researchers will be in attendance.

Russell Judge, NASA/MSFC, Huntsville, AL

I am very grateful for the travel award. To me, principally going to the Glasgow meeting was an excellent opportunity to know the different trends in research in crystallography around the world and the most interesting topics at the present; also to learn different aspects, applicability, limitations and advances in the techniques to study all kind of crystalline solids. It was also very useful for updating specific information (like computer programs, bibliography, internet sites, courses, equipment, etc.).

Silvina Pagola, Brookhaven National Lab, Upton, NY

I am happy to write to you about my attendance at Glasgow. I find it especially fitting since I see that your computer is named harker—I assume after David Harker—because the work I presented at IUCr'99 is partly an extension of Harker's work on color symmetry to quasiperiodic crystals.

Getting an invitation to speak at one of the micro-symposia at the IUCr Congress was a great opportunity for me for two very different reasons. First, it allowed me to interact with the experts in my field regarding recent advances in our research, both by attending each other's talks, as well as through informal conversations between the scientific sessions. But even more importantly, a conference such as this brings together scientists with diverse backgrounds in crystallography. This allowed me to present my work on the symmetry of quasiperiodic crystals to a much wider audience than I would normally get in a more specialized meeting. I find that more than 15 years after the discovery of the first quasicrystal there is still an air of mystery, at least among non-specialists, regarding the understanding of their symmetry. I hope that I managed to relieve some of that mystery for the people who attended my talk.

As I said, my research deals with the symmetry of quasiperiodic

crystals (<http://www.cmp.caltech.edu/~lifshitz/>). In particular, I've developed my own theories of color symmetry and magnetic symmetry for quasicrystals. My talk at IUCr'99 was a review of the former. I was a graduate student of David Mermin at Cornell University from 1990-1995 where I learned about the symmetry of crystals. Since 1995 I've been a postdoc at Caltech, where I worked independently on my theories of color and magnetic symmetry.

I cannot thank the US National Committee on Crystallography enough for giving me a travel award to attend the IUCr Congress. Without their support I would not have been able to attend the conference. Period. As a postdoc, I have no funds of my own and my efforts during the last two months to obtain partial support from Caltech to cover the rest of my expenses have been completely in vain.

Ron Lifshitz, California Inst. of Tech., Pasadena, CA

The support provided to me by NASA made attendance at this meeting possible and gave me the opportunity to present my work on the ultrahigh resolution crystal structure of Endonuclease IV and its complex with damaged DNA. The positive experience I gained in presenting this research to international experts in crystallography, biochemistry, and biophysics provided me with excellent opportunities to meet these scientists and gave me ideas on experiments designed to expand on present results. Furthermore, interaction with small-molecule crystallographers gave me important insights into how some of the methods currently used in the small-molecule field may soon be applied to macromolecular crystal structures. A particularly valuable personal benefit derived from attending the IUCr meeting in Glasgow was the opportunity I had to attend presentations by potential post-doctoral supervisors. As I am currently in the final stages of my doctoral research program the opportunity to not only attend these presentations but also to discuss potential projects in a relaxed setting gave me solid ideas as to the fields of research that I plan to pursue in the near future.

David Hosfield, The Scripps Research Inst., La Jolla.

I participated fully in the technical sessions in the XVIIIth IUCr 1999 Congress. The attendance of the IUCr 1999 in Glasgow enabled me to present my work "Crystal Structure Solution of Compound Semiconductor $\text{Cu}_3\text{In}_7\text{Se}_{12}$ from Combined Convergent Beam Electron Diffraction, X-ray Powder Diffraction, and X-ray Absorption Fine Structure Data". There were plenty of opportunities for extensive discussion with other attendees, especially during the poster sessions. Representation at the conference was international. I was able to see the strong development of crystallography in other areas of the world.

I also attended the workshop "Electron Crystallography". The discussion in the workshop was intensive. Many leading researchers in this field were participating in this workshop. I certainly have learned the most recent developments and available techniques for doing research.

Many excellent talks and posters enhanced my understanding of crystallography and helped me learn new techniques to study

my research problems. Of course I enjoyed very much the trip to the beautiful Arran isle for the day off. The trip is truly fruitful and I am truly grateful for the financial support from USNCCr.

Chih-hung (Alex) Chang, U of Florida, Gainesville, FL

I am working on Data Processing Suite (www-dps.bio.purdue.edu). DPS will be a complete package for processing single crystal X-ray diffraction data of proteins, viruses, nucleic acids and other biological complexes. The emphasis is on data collected at synchrotron radiation sources. The programs are provided free of charge.

Without the Travel award I would not have been able to attend the IUCr meeting in Glasgow. Apart from the many excellent presentations, I would have missed the many discussions with leaders in the field of data processing and the many discussions with users of data processing packages.

The presentations and discussions at the IUCr meeting gave me an understanding of the needs and desires of scientists using data processing packages. It also provided me with clear ideas for new strategies and improvements of current data processing packages. I am looking forward to providing the crystallographic community new data processing programs that are, in large, based on my experiences in Glasgow.

Kai van Beek, Purdue University, W-Lafayette, IN

Currently I am a 5th year graduate student at The Scripps Research Inst.. The focus of my thesis work is the determination of the 3-D crystallographic structures of abalone fertilization proteins and subsequent analysis of these structures for insights into the biological roles and mechanisms of these proteins. Specifically, I work on abalone sperm lysin and its egg receptor VERL. Lysin is a protein located in the abalone sperm and it is involved in initial species-specific interactions with the egg and it also creates a hole in the egg's protective coating through which the sperm can swim. VERL is the egg receptor for lysin. So far, I have refined the structure of lysin from one species of abalone and determined the novel structure of lysin from another species of abalone. Currently, I am working on solving the structure of the complex of lysin and VERL.

Attending the IUCr gave me the opportunity to meet with other people involved in the crystallography of fertilization proteins and to discuss our projects and methods. The conference also provided an opportunity to learn about novel techniques that I could apply to my research. And of course, I also got to find out about interesting new structures that had been solved as well as new instruments and synchrotron sources. Most importantly, the conference allowed me to meet a variety of crystallographers from all around the world. These new contacts will surely come in handy in future collaborations or in just providing help with problems which I cannot solve myself. At this point in my career I am also starting to look for postdoctoral positions, and I was able to meet several potential employers.

So, overall, attending the IUCr in Glasgow was extremely beneficial to me both in my current and future endeavors.

Nicole Kresge, The Scripps Research Inst., La Jolla, CA

I am writing you to express my appreciation for the grant I received from the USNCCr and NASA that allowed me to attend the IUCr XVIII Meeting in Glasgow, Scotland last month. My research is in the area of EF-hand calcium-binding proteins and I presented a poster with several crystal structures of parvalbumin mutants. I met several groups from different countries that also study the structure and function of EF-hand proteins at the conference. There were two groups from Sweden and one from Japan that I talked with extensively, and I thought it was very exciting to have the opportunity to discuss research with individuals that I would never otherwise have a chance to meet.

The lectures that I attended were quite excellent. I also attended one of the workshops (the CCP4 workshop) and I thought that it contained a lot of practical information.

As I am a graduate student in the Department of Biochemistry at Rice University, attendance at this meeting would not have been possible without the joint USNCCr and NASA grant.

M. Susan Cates, Rice University, Houston, TX 77005

The meeting in Glasgow was the second IUCr meeting I attended and the main benefit for me was the interaction with other scientists, former colleagues as well as new people working in related fields. In addition to presenting my work in form of a poster, I have co-organized a computer simulation workshop with Prof. Neder (U Wuerzburg, Germany). A pleasant observation for me was the growing interest in diffuse scattering and defect structures which was reflected by a plenary lecture by T.R. Welberry and a dedicated microsposium as well as talks and posters in other symposia. Since this is the area of crystallography I am working in, there was plenty of opportunity to exchange ideas. As a consequence a significant part of my 'projects-to-do' list is a direct consequence of attending the meeting in Glasgow. As a post-doc the meeting was also a great place to hear about possible job opportunities. Last but not least I have very much enjoyed visiting Scotland and Glasgow.

I would like to thank the US National Committee for Crystallography for the travel grant which made my travel to Glasgow at all possible.

Thomas Proffen, Michigan State University, East Lansing, MI

I am a graduate student who received an award from USNCCr to travel to Glasgow for the 1999 IUCr meeting.

Being a physicist and the only person in my lab working on biological crystallography, going to the IUCr meeting allowed me to witness more of the crystallographic community. I became aware of issues that interest mainstream members of the community. It helped put my research in context.

A pleasant surprise was how the conference encouraged multi-disciplinary research, both across subject matters and across experimental techniques. For example, there were talks on neutron scattering and electron microscopy, and how they complement crystallographic techniques. Also, the plenary lectures were all timely, and had more of a tutorial feel.

The travel award also allowed me to give a talk on high pressure macromolecular cryocrystallography during the “High Pressure Studies of Biological and Other Soft Matter” (110C) microsposium.

I am grateful to USNCC for this opportunity. Thank you.

*Paul Urayama, Cornell University, Dept of Physics,
Ithaca, NY*

I was very fortunate to receive funding towards this conference. It was a wonderful experience because I got to meet a lot of people from all over the world who are involved in crystallography and as a result I have made a few contacts who may be useful in finding a job later in my career. I presented a poster and received interesting comments concerning my work: although the poster sessions were a little short and at lunch time. I also talked to other people working in similar areas but didn't get to meet as many people as I hoped: there was only one 'student' event which was sold out before I arrived. Some of the other events were too expensive and there wasn't much else scheduled in the evenings. The microsypmposia were very interesting. In fact I didn't get as much free time as I hoped! The majority of the speakers were very good. They spoke within their time allocated and their talks actually were relevant to the session.

I also obtained several computing packages that I could download from the web and details of other software developments which was important since commercial packages can be very expensive.

Overall it was very enjoyable and worthwhile.

Dianne Ellis, Baylor University, Waco, TX

Attendance at the 18th IUCr meeting, in Glasgow, was a great success from my perspective. Meetings such as this one allow researchers the opportunity to present their research as well as to see cutting edge research first-hand by colleagues from all over the world. The Travel Awards are particularly important for scientists fairly early in their careers as they usually do not have their own resources to attend meetings in international locations. It is much easier to convince your supervisor or department chair to support attending this type of meeting when he/she is not paying the total cost of the trip. The meeting in Glasgow was very helpful in staying current in research in crystal growth, making contacts which will lead to fruitful collaborations, and generating new research ideas for future projects. My thanks to the ACA and sponsoring agencies for their supporting me and other scientists at this meeting.

*Terry L. Bray, University of Alabama at Birmingham,
Birmingham, AL*

The travel award enabled me to attend the IUCr meeting in Glasgow and present a poster on my research. I also attended sessions on electron microscopy applied to crystallography and structural biology and also protein crystallography and *ab initio* phasing. I am currently involved in single particle reconstruction (from electron micrographs) and relevant lectures by some of the major researchers in this field indicate that this method is becoming important for providing a starting phase set (for phase extension of X ray diffraction data) for large protein complexes and also for low/ medium resolution structure determinations for icosahedral viruses.

*William Nicholson, Lawrence Berkeley Laboratory,
Livermore, CA*

Cover Story

The scenes of Saint Paul were kindly provided by the Saint Paul Convention and Visitors Bureau (www.stpaulcvf.org) and the Saint Paul River Centre (www.rivercentre.org). The meeting logo was originated by the local committee in Saint Paul and “rendered artistic” by Patti Coley.

The photo at the top left is a view of Saint Paul as it sits high on the bluffs above the Mississippi River. Top right shows the Landmark Center which was dedicated in 1902 at the Federal Court House. It now houses programs for visual and performing arts and civic activities. In the lower left corner is the Cathedral of Saint Paul which is modeled after Saint Peter's Cathedral in Rome. It was dedicated in 1915 by Archbishop John Ireland as a monument to the people of Saint Paul. In the lower right is the Josiah Snelling Paddleboat which is one of two sternwheeler riverboats that provide excursions and dinner cruises on the Mississippi from May through October. On both sides in the middle are two views of the Saint Paul River Centre which will be the venue for the scientific sessions for the ACA meeting.

The 58th Pittsburgh Diffraction Conference, Columbus, OH, October 21 - 23, 1999

The 58th PDC was held at the Parke University Hotel on the edge of the Ohio State University campus in Columbus, Ohio. This year there were two symposia. The first, organized by George DeTitta was entitled "The Physical Properties of Protein Crystals". The second, organized by Martin Caffrey and Bryan Craven, was entitled "From Nucleic Acids to Proteins" and was held in honor of Muttaiya Sundaralingam, Ohio Eminent Scholar and Professor of Chemistry at The Ohio State University. A session consisting of 17 posters was organized by Patrick Woodward, who also did an excellent job in making local arrangements for the conference. The scientific sessions had 85 attendees, including many members past and present from Sunda's research group. They came from India and Japan, France and Germany and from academic, government and corporate institutions all over the United States.

The Conference Awards Committee was made up of Steven Geib and John Rosenberg for judging the Sidhu Award and they were joined by William Duax for judging the Chung Soo Yoo Award. This year two Sidhu Awards were made for outstanding contributions to crystallography and/or diffraction by scientists within five years of completing the PhD. These went to Drs Changill Ban from NIH and Markus Wahl from the Max-Planck-Institut für Biochemie, Martensreid, Germany. The Chung Soo Yoo Award for the best poster by a graduate student went to Yong Xiong from OSU. It seemed appropriate that this year all three awardees were or are students of Sunda.

The Conference Dinner provided a convivial evening, but one saddened by the absence of George Jeffrey, who as scheduled Master of Ceremonies, was unable to attend because of illness. Jeff sent his best wishes to all conferees. In return, the conferees signed a copy of the Conference Program containing a message for Jeff expressing their regrets. His place was taken by Bryan Craven, one of those present four decades ago when Sunda arrived in Pittsburgh to begin his studies of X-ray crystallography

under Jeff's guidance. Others at the dinner who remember Sunda's arrival were Ryonosuke Shiono and Dick McMullan.

After obtaining his PhD at the University of Pittsburgh in 1961, Sunda joined Lyle Jensen for a postdoctoral term at the University of Washington. It was during this time that Sunda began his study of nucleic acid structure. In 1965 he moved to Bob Langridge's lab at Children's Hospital in Boston before accepting his first faculty position in 1966 at what was soon to be Case-Western Reserve University in Cleveland. In 1969 he moved as a full professor to the Biochemistry Department at the University of Wisconsin. At Madison, Sunda and his group became involved in the macromolecular crystallography of nucleic acids (tRNA) and proteins (troponin C). He also established his reputation as an authority on the stereochemical principals important for determining the conformation of nucleic acids, phospholipids and carbohydrates. Thus he advanced the concept of the "rigid" nucleotide. After twenty years at Madison, Sunda accepted the Ohio Regents Eminent Scholar Chair and became Professor of Chemistry at The Ohio State University in Columbus, where he has continued his work on proteins and DNA and RNA oligonucleotides. He now has about 330 published papers.

At the dinner, after the Awards were presented, Yathindra came forward to wrap Sunda in a most handsome shawl. In this traditional ceremony, Yathindra was assisted by Herb Hauptman. Throughout the evening, other colleagues and former students paid tribute and told stories of their years with Sunda. Doug Rohrer spoke of the early days at Cleveland. Dave Stout and Stephen Sprang talked of their student days at Madison. The three awardees (Markus Wahl, Changill Ban and Yong Xiong) expressed gratitude for their experiences at Columbus. Bi-Cheng Wang, a long-time colleague, remembered his collaboration with Sunda on the structure of troponin C, which was an early success for the solvent-flattening method. Finally, Bob Bergstrom and Gale Strasburg (ex-Madison), produced an elegant rocking chair. This was presented to Sunda on behalf of former and present members of Sunda's research group.



Members of the Sundaralingam research group, past and present.: Front row (from left): J. Deng, K. Shi, S. Sprang, S. N. Mitra, M. Sundaralingam, X. Chen, B. Pan, S. Vasudevan, B. Burkhart. Second row: J. R. Rubin, R. K. McMullan, S. T. Rao, E. Westhof, H. Mizuno, N. Yathindra, C. Sudarshanakumar, Mrs R. Biswas, D. Tippen. Third row: Y. Xiong, M. Sabat, B. Ramakrishnan, R. Bergstrom, E. Merritt, Z. Lin, K. Balendiran, C. Ban, M. C. Wahl. Fourth row: K. Satyshur, R. G. Brennan, C. D. Stout, R. Bott, D. C. Rohrer.

The Poster Session.

The 17 posters were displayed throughout the meeting but were the focus of attention at the mixer. Most posters were related to the topics of the two conference symposia. There were four posters from Martin Caffrey's group at OSU that dealt with the structures and phase equilibria of lipid mesophases and the use of lipid mesophases in assisting crystallization of membrane proteins. These were presented by V. Cherezov, X. Ai, D. Siegel and Y. Misquitta. Posters on protein physical properties and protein crystallization were presented by Anna Holmes (University of Alabama in Huntsville) and John Petock (Thomas Jefferson University). Alan Pinkerton described an open flow helium cryostat for macromolecules which has been developed at the University of Toledo. The instrument could be used for neutron and macromolecular X-ray data collection. Crystal structure determinations were described for a domain of a 5S RNA with a cytosine bulge in one strand (Yong Xiong, OSU) and a fragment of virus reverse transcriptase complexed with a pseudo-16-mer DNA in which there are G-A mispairs (Marie Coté, Rutgers University). Jianhua Fu (Stanford University) described results in the phasing of a very large protein (RNA polymerase II) by using heavy atom clusters. High resolution crystal structures of archeal histones were presented by Kathleen Sandman (OSU). Other protein structures reported were the ribonuclease colicin E3 which acts as an antibiotic (M. Shoham,



Xiong Yong with the poster that won him the Chung Soo Yoo Award. Changill Ban and Bill Duax look on.

Case Western Reserve University) and hypoxanthine phosphoribosyl-transferase (G. K. Balendiran, Texas A&M University). The absence of HGPRase activity is linked with mental retardation and hyperuricemia. Kenneth Satyshur (University of Wisconsin) described the crystal structure of the aspartic protease rhizopuspepsin and showed that various inhibitors were bound as predicted by the Growmol computer program. There were three posters involving inorganic structural chemistry. Michael Lufaso (OSU) presented results obtained using the computer program SPuDS which predicts the nature of the perturbation of the simple cubic perovskite structure as a result of changes in chemical composition. Jianping Liu (OSU)

described the synthesis and X-ray crystal structures of two families of cyanide-bridged lanthanide-transition metal complexes. Representatives of the two families have the same empirical formula but they differ in chemical structure. Charles Lake (Indiana University of Pennsylvania) reported the crystal structures of a series of organometallic molecules containing both group 13 and group 15 elements. These materials are being designed to improve the characteristics of thin-film semiconductors.

Symposium: The Physical Properties of Protein Crystals.



Participants in the Symposium on the Physical Properties of Proteins. Front row (from left): George DeTitta, Anna Holmes, Heather Volz, Gloria Borgstahl, Dick Matyi. Back row: Chris Yip, Bob Blessing, Eddie Snell, Arunan Nadarajah, Rob Thorne, Yuri Kuznetsov.

A session on protein crystals as subjects of materials science centered on tools as diverse as atomic force microscopy (AFM), X-ray topography, high resolution diffraction and mechanical bending. These were used to describe objects that are interesting in ways quite apart from their biological importance. As anyone who has mounted a protein crystal for diffraction can attest, these are objects quite unlike their small molecule siblings. Bob Blessing (Hauptman-Woodward Institute) described the prospects for the experimental determination of the charge density distribution in protein crystals using ultra-high resolution X-ray diffraction methodologies. Anna Holmes (University of Alabama in Huntsville) has subjected crystals of lysozyme to mechanical stress and measured their Young's moduli. Eddie Snell (Marshall Space Flight Center, Huntsville) and Rich Matyi (University of Wisconsin) concentrated on what information could be extracted from rocking curves of diffraction maxima taken with highly parallel X-ray beams, either at synchrotron beam lines or now, most impressively, at home with four-bounce monochromators. Rob Thorne (Cornell University) showed by way of X-ray topography what differential growth conditions do to crystal long range order. In the AFM section of the session, Arun Nadarajah (University of Toledo) did double duty, presenting work on growth mechanisms of lysozyme uncovered both by his group and by Mary Ann Perozzo and John Konnert (Naval Research Lab), who at the last moment were unable to attend. Yuri Kuznetsov (UC Irvine) elegantly showed how crystal growth is a complex, untidy affair, demonstrating how impurities and crystalline debris can incorporate into growing faces. Chris

Yip (University of Toronto) showed what AFM can teach us about biologically important crystallization/dissolution processes, such as the release of insulin from its crystal structure. The participants came away with a richer picture of those objects we too often see as a means to an end (a beautiful structure) but which in themselves are interesting objects.

Symposium: From Nucleic Acids to Proteins.

This symposium in honor of Muttaiya Sundaralingam's first forty years in X-ray crystallography was prefaced by remarks from Bruce Bursten, Chair of Chemistry at The Ohio State University. After making us welcome, Bruce revealed himself as one of us, because in earlier days he determined a number of inorganic crystal structures. Martin Caffrey, also from the Chemistry Department at OSU, contributed much to the organization of this symposium but could not attend because he was on leave. The Chair was taken by Bryan Craven. There was especially rousing applause on two occasions during the symposium. The first came almost immediately when Sunda, as first speaker, announced that he was celebrating his birthday. The other came as Eric Westhof began to speak and Sunda announced that Eric had newly been admitted to the French Academy of Sciences.



M. Sundaralingam wearing his ceremonial shawl

Sunda presented a masterly overview of the observed hydrogen bonding interactions among the four bases adenine, thymine, cytosine and guanine when they are taken in all ten pairing combinations, including the self pairs. He emphasized the variety of pairing modes, sometimes mediated by water molecules, which occur when an oligonucleotide chain forms mismatches or bulges and when two or more chains interact.

The next speaker was Herb Hauptman (Hauptman-Woodward Institute) who answered "Yes!" to the question whether 100% success is possible for the Shake-and-Bake method of phasing large structures, including lysozyme. Success is achieved if accurate data of sufficiently high resolution are available. Additional exciting news for determining large structures came from Bi-Cheng Wang (University of Georgia) who reported success with two proteins (48KDa with 4 iodines;

84KDa with 4 irons) from single-wavelength anomalous scattering data collected in-house. Solvent flattening methods were used. Ethan Merritt (University of Washington) reviewed developments in obtaining realistic anisotropic thermal displacements for resolved atoms in protein structures. These three speakers, together with Bob Blessing in the first symposium, illustrated how the improved accuracy now being obtained for protein X-ray data is opening the way for important new opportunities.



Mert Adams with Herb Hauptman. Sadly, this may have been the last crystallographic meeting where Mert represented the Polycrystal Book Service. Herb arrived at the meeting directly from a lecture tour of Ireland.

Helen Berman reported on the formation of the Research Collaboratory for Structural Bioinformatics (RCBS), which incorporates structural data from the Protein Data Bank, the Nucleic Acid Database and the Cambridge Structural Database. The RCBS represents a partnership of Rutgers University, UC San Diego and NIST. Helen was loudly applauded after a comment from the floor that great progress had been made both scientifically and in dealing with delicate political matters.

Brian Burkhart (Hauptman-Woodward Institute) talked on the pentadecapeptide gramicidin D that forms biomembrane channels specific for monocations. From a body of crystal structural data, extrapolations were made about how the pores function. These have raised a storm of protest in the scientific weeklies which has not yet subsided.

Four speakers addressed the structures of nucleic acids. N. Yathindra (University of Madras) described the alternate world in which nucleotides have 2',5' linkages rather than the 3',5' linkages favored in nature. The alternate world also allows formation of A, B and Z duplexes. Yong Xiong (Ohio State University) reported the crystal structures of two oligonucleotide DNA:RNA complexes. These contain only pyrimidine bases in the DNA strand and purines in the RNA strand. The duplex has the A-conformation. While normally such hybrid complexes are hydrolyzed by RNase H, the polypurine tract is stable, possibly because it adopts the A structure with enhanced stability owing to base-stacking. David Stout (Scripps Institute) talked on DNA enzymes that catalyze site-specific cleavage of RNA. He presented some remarkable structures, for example, a 108-nucleotide having

two strands of DNA and two strands of RNA. The crystal complex contains five double-helical domains and exhibits four-way junctions. These junctions have different conformations in different crystal complexes, thus providing insight into the flexibility of the Holliday junctions. Eric Westhof (IBMC-CNRS, Strasbourg) surveyed experimental and theoretical studies on the folding of large catalytic RNAs. The hierarchy of folding begins with the pairing of strands, then the stacking of helices and finally the association of helical domains into bundles stabilized by RNA-RNA interactions. There is repeated use of two types of long-range RNA-RNA anchors, namely GNRA tetraloops with their receptors and loop-loop complementary interactions. RNA structural motifs found in small ribozyme systems are recurrent in large ribosomal RNAs.



Presentation of the Sidhu Awards by (from left) Steve Geib and John Woolcock (Past-president and President, Pittsburgh Diffraction Society) to Markus Wahl and Changill Ban.

John Rosenberg (University of Pittsburgh) reported new studies of the DNA-Eco RI crystal complex at 1.8Å resolution. Unexpectedly, substitution of purine (adenine sans amino group) for adenine in the recognition sequence leads to higher DNA-protein binding affinity. From the detailed structure, John suggests that the substitution allows the thymine that is paired with purine to form a stronger thymine-protein hydrogen bond. This talk was followed by the two Sidhu Lectures, which both involved the structure determination of a protein that functions by interacting with nucleic acid. Markus Wahl (Max-Planck-Institut für Biochemie, Martensried) described the crystal structures of two forms of the large L12 ribosomal protein. In both forms, the asymmetric unit consists of two complete L12 molecules and two N-terminal fragments and contains a noncrystallographic twofold axis. The dimerization modes (different from those previously proposed) may also occur *in vivo* and *in situ*. The other Sidhu Awardee, Changill Ban (NIH, Bethesda), reported the structure of the 40KDa N-terminal fragment of the protein MutL. This protein initiates methyl-directed DNA repairing in *E. coli*. The crystal structure was determined together with complexes containing a substrate analog (ADPnP) and the reaction product, ADP. This work strongly indicates that MutL is an ATPase. ATP binding seems to involve protein dimerization and significant conformational changes. Two other speakers described proteins that function via interaction with nucleotides. Stephen Sprang (University of Texas

Southwestern Medical Center, Dallas) discussed nucleotides as regulators and signal transducers. He has helped in the understanding of a linked signalling network by carrying out the crystal structure determination of protein kinase A, one of its targets, namely the catalytic subunit of glycogen phosphorylase kinase and also glycogen phosphorylase itself. Janet Smith (Purdue University) described studies of a protein structural family that has become adapted for catalytic and regulatory functions. This family contains the phospho-ribosyl-transferase (PRT) fold which can adapt to bind nucleotides and related compounds that have a ribose-5-phosphate group. Janet advanced a mechanism for the phosphoryl transfer reaction based on the crystal structures of a number of PRT proteins complexed with substrate and product analogs.

B. Ramakrishnan (NCI-FCRDC, Frederick) spoke on a family of six β-1,4-galactosyltransferases which have a high sequence homology. These tissue-specific enzymes are essential for oligosaccharide synthesis but, owing to incomplete crystal structural data, their structure-function relationships are not well understood. Hydrophathy plots similar to those used for identifying the membrane-binding region of membrane proteins have been useful for identifying the sugar binding region of the Gal-T enzymes. Hiroshi Mizuno (National Institute of Agrobiological Resources, Tsukuba) described the crystal structure of a complex between the coagulation factor X-binding protein and a 44-peptide fragment containing the Gla domain. He showed that the GD binding site, similar to that of prothrombin fragment 1, contains seven bound calcium ions, one of which interacts with the X-binding protein. Richard Brennan (Oregon Health Services University, Portland) has determined the crystal structure of the drug-binding domain of the multidrug transporter, BmrR and also its crystal complex with a tetraphenyl-phosphonium drug. A drug-induced protein unfolding and the relocation of an α-helix exposes an internal drug pocket with a buried glutamate. This helps explain why BmrR binds numerous hydrophobic cationic drugs.



Symposium organizers Bryan Craven and George DeTitta have a chuckle with Monica Niederhut.

This symposium was a testament to the high scientific standards and the personal example set by Sunda over the years. His legacy is that so many former members of his research group are now producing outstanding work.

George DeTitta and Bryan Craven

USNCCr Meeting, Washington, DC, November 14, 1999

The U. S. National Committee for Crystallography (USNCCr) held its second meeting of the year on Sunday, November 14, 1999 at the National Academy of Sciences Building in Washington, DC. In attendance were: (back row) Bill Duax, Dick Harlow, Peter Buseck, Jim Kaduk, Mark Rivers, Lonny Berman and Ian Robinson: (front row) Alex Chernov, Abe Clearfield, Tamae Wong, Cele Abad-Zapatero, Gary Gilliland, Charlie Prewitt, Jane Griffin and Bob Sweet: (seated) Connie Chidester, Marv Hackert, Judy Flippen-Anderson and Bing Jap: (missing) Lee Brammer, Howard Einspahr and Cyndy Stauffacher. Bing Jap (Lawrence Berkeley Lab) is new to the Committee and Bill Duax has returned as an ex-officio voting member due to his status as a newly elected member of the Executive Committee of the IUCr. Leaving the Committee at the end of the year will be Cele Abad-Zapatero, Lonny Berman, Dick Harlow, Mark Rivers and chair Judy Flippen-Anderson. Marv Hackert will assume the chair in 2000 and the Committee will welcome new members Charlie Carter (University of North Carolina), Jon Clardy (Cornell), Steve Ealick (Cornell) and Winnie Wong-Ng (NIST).



The highlight of the meeting was a visit from Art Bienenstock who is currently serving as Associate Director for Science at the Office of Science and Technology Policy (OSTP) as a political appointee. He is on leave from Stanford, and expects to return there at the end of this administration. He started the discussion by giving us a general overview of what OSTP does and how he fits in to the overall picture: Neal Lane serves as the President's science advisor and the head of OSTP. The four sections of OSTP are National Security and International Affairs, Environment, Technology, and Science. Bienenstock heads this last section, which has nine professional staff. The Science section works closely with OMB trying to get science budgets increased. Their goal is to achieve balance between NIH (and keep it healthy) and the rest of science. Over the last 30 years, the GDP has increased by 122%. The NIH budget has increased by 160% (roughly in line with the GDP), while the physical sciences have seen their budgets increase by 20%, and engineering by only 2%. These increases mean that the physical sciences are "falling behind". This trend has been steady, and independent of the party in power. This year, the President's budget proposals had a larger increase for physical sciences than NIH, but Congress increased the NIH budget.

The framework for the government/university research partnership changed in the late 80s/early 90s. These changes led to the introduction of a lot of accounting, and to a net transfer of costs from the government to the universities. The Science

section is trying to decrease the strain between the government and universities, and has issued a report on the principles and practices of research (Neal Lane, *Academic Medicine*, April 1999). This report concludes that research is a long-term investment, and that research and education are integrally linked. Bienenstock's office is holding a series of workshops with universities, and is trying to alter some of the documents which govern the government/university relationships.



Art Bienenstock

There is a large interagency effort aimed at encouraging participation of women and minorities in the scientific workplace. If more women and minorities do not enter the scientific workforce, the number of H1B visas will need to be increased to keep the fraction of the overall workforce in science and technology increasing. Over the last 20 years, the number

of white males in the S&T workforce has decreased by 40,000, while the number of women, minorities, and H1B visas has increased by 20,000. The current unemployment rate of B.S./technicians (non-Ph.D.) is 1.4%.

The Science section of OSTP works on policies for genetic

engineering. The controversy on cloning and work on stem cells is relatively quiet now, but occasional efforts are made to stop federal funding for such work.

The DOE and NSF originally funded national user facilities such as synchrotrons, and only later did NIH-funded research become important at these facilities. Bienenstock noted that DOE and NSF continue to have the responsibility for operating costs, but are sensitive to the needs of NIH. OSTP has helped to obtain increased funding for the synchrotrons - leading to more staff at SSRL, NIH-funded beamlines at all facilities, and upgrades to NSLS and SSRL.

After Art finished his remarks there was some discussion about the status of HFBR at BNL and whether or not it would ever get restarted but this became moot when Secretary of Energy Richardson announced a few days later that the HFBR at BNL will not be restarted. There was also a lively discussion regarding current attempts to patent crystal structures and coordinates. The concern was raised that chemists are driven by what is not patented, and that the issuance of a patent could mean that whole areas of research are "prohibited" or discouraged. Questions were raised about what it really means to patent a structure and whether a structure should be considered an invention (which should be patentable) or a discovery (which should not be patentable). The general consensus was that this is one issue that will ultimately be resolved in the courts.



Incoming USNCCr Chair Marv Hackert (UT Austin) and new member Peter Buseck (Arizona State)

A comment about the frightening "Kansas situation", where the State Board of Education has made the teaching of evolution optional turned the discussion toward education in general and to attracting bright students to science and to science teaching in particular. Marv Hackert described a program at the University of Texas in which freshmen are paired with local schools, serving as teaching interns. About 200 students are involved currently. After a discussion of the importance of early science education, Bienenstock noted that college is not too late to excite students' interest; his own experience demonstrates that students can get

excited about science in college and that undergraduate research experience is especially critical. He emphasized that non-university (industry and national laboratory) scientists should consider offering undergraduate students research opportunities.

After Art left the meeting returned to business as usual and the Committee heard reports provided by the representatives of the ICDD (Charlie Prewitt), the American Association for Crystal Growth (Alex Chernov), and the Microscopy Society of America (Bob Glaeser) about what is happening in their organizations.

We were filled in on what's happening at the various databases of interest to crystallographers by Connie Chidester who chairs the Database Subcommittee. Gary Gilliland also gave a short report on the current status of the PDB indicating that the transition from Brookhaven to the new collaboratory (Rutgers, NIST and SDSC) was completed three months ahead of schedule partly due to the excellent cooperation received from the Brookhaven staff. (For an update on the PDB see page 6).

Mark Rivers (chair of the Research Resources Subcommittee) gave an excellent update on the status of the various high energy resources around the nation. Ian Robinson (chair of the Education Subcommittee) described their attempts to put together a list of crystallographic courses offered at US universities. Jane Griffin reported on the successful travel award program for Glasgow (see pages 16-21 for more details). Then Abe Clearfield rounded out the meeting with an update on ACA activities.

Jim Kaduk, Secretary

10th Annual Southwest Macromolecular Symposium, Texas A&M University, College Station, Texas, November 19-20, 1999

For the past 10 years, protein crystallographers around the state and from the southwest have traveled annually to central Texas to present their results and meet fellow crystallographers. This year, the format was expanded to include four invited speakers. Bob Sparks, Johann Deisenhofer, Keith Moffat, and Michael Rossmann. For titles and abstracts, see: <http://cmdnmr.tamu.edu/meyerlab/mlab/swms/swms.html>

Bob Sparks (Bruker AXS) described crystallographic computing before the advent of computers and how their availability influenced the powers of the method, using his work with the structure analysis of vitamin B₁₂ as an example. He showed how hardware and software have changed how we think and work. He predicted that CCD data will replace synchrotron data for more routine studies and that increasingly, no one will know the code inside 'black-box' software.

Keith. Moffat (U. of Chicago / APS) described the results of his study of two protein systems on the nanosecond time scale, CO-myoglobin and 14kDa PYP, the blue light absorbing Photoactive Yellow Protein. He presented impressive 'movies' of the time-dependent relaxation of the haem group upon release of ligated CO and photoinduction of PYP. There was considerable interest from the group about the application of these methods to study rapid chemical processes, possibly into the picosecond range.

Michael Rossmann (Purdue) presented studies at 25Å resolution on the structure of viral receptors and viruses, using polio virus and related viruses as examples. These complex structures have been determined using a combination of electron microscopy and X-ray diffraction. Results show the presence of a deep “canyon” in the center of the viral asymmetric unit that corresponds in shape and orientation complementary to extracellular recognition factors.

Johann Deisenhofer (HHMI, UT Southwestern Medical Inst.) described the structural analysis of a 665 amino acid bacterial nucleotide excision repair (NER) enzyme which progressed from finding crystals to a draft of the paper in under 6 weeks. This is an example of the powers of the crystallographic method, coupled with an effective expression system. He then reflected on the increasingly dominant role structural genomics appears to be playing in influencing the choice and initiation of structural studies. He then described the laborious structural analysis of neurexin 1b, which helps target neuron synaptic connections, suggesting that such studies might not be as common in the future because of the difficulties involved and the uncertainty of positive results for the efforts. Finally, he made a case for the continued emphasis on crystallography as an academic and scientific discipline that should be taught (and learned) systematically rather than coincidentally.

Thanks to generous support from commercial contributors, it was possible to keep registration costs to a minimum and still enjoy a buffet dinner in the evening, followed by presentations by two who were there when it happened. F. Albert Cotton described the events leading up to Lipscomb’s structural analysis of carboxypeptidase A while he was on the MIT faculty, including photographs of former students and a view of a Richards’ box, which most younger (even middle-aged?) crystallographers have heard described only in mythical terms or as part of the recitation of a saga or epic. He then described how he and E.E. Hazen started the study of Staph. nuclease, which they brought with them to Texas A&M in 1972 and completed several years later, making it the first protein to be modelled into density in 3-D on a computer, using program FIT in Edgar Meyer’s lab.



Keynote speakers + organizer: left to right: Johann Deisenhofer, Edgar Meyer, Michael Rossmann, Allen Edmundson, F. Albert Cotton, Keith Moffat, and Robert Sparks.

Allen Edmundson described how, as a graduate student at the Rockefeller Institution, he was given the project of determining

the sequence of sperm whale myoglobin, subsequently going to Kendrew’s lab to help with its crystallographic analysis. Reinforcing Bob Spark’s talk, he had photographs of the computing methods of the 1950s, as well as a number of photographs of predecessors and contemporaries who contributed to the research. He shared lab and office space in Cambridge with Michael Rossmann, who was in Perutz’ group studying haemoglobin. Following an excellent dinner, the warmth and wisdom of the several contributors to the early days of protein crystallography gave balance to the day’s proceedings and greater perspective to a theme of the symposium: views past, present, and future.



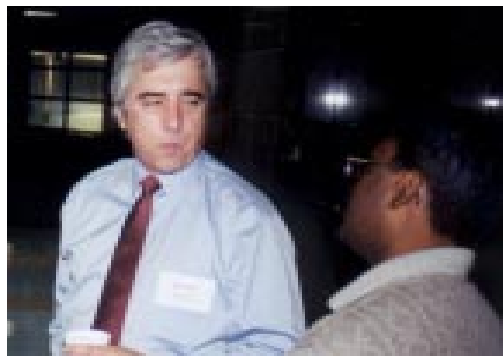
Jonathan Friedman (U. of H) discusses an approach to phasing with Wah Chiu (Baylor), who gives more phases than he receives.

The following day was devoted primarily to presentations by students and post docs from Dallas, Galveston, and Houston. Exceptions included a presentation on the use of structural genomics in the bio-tech industry (Peat & Newman). Kris Tesh presented recent developments in methodology at the Molecular Structure Corp. (founded in 1974 in College Station). Edgar Meyer showed some new, solid (wooden) molecular models that are derived from computer graphics but have greater similarity to the earliest (e.g., Kendrew) models.



Coffee break: Stephen Ernst, Marvin Hackert, Edgar Meyer, Stan and Rosie Swanson are planning next year’s symposium – or something more insidious?

And then, there was the second reason for a grand celebration: the initiation, funding, staffing, and establishment of a regional MAD beam line at the LSU synchrotron, CAMD, represented by Ben Craft and Josef Hormes, Director of CAMD. The idea for this beamline originated (Marv Hackert) at one of the first of these symposia and was nourished and brought to fruition by an ad-hoc steering committee consisting of Bob Fox, Edgar Meyer, and George Phillips, who now chairs the consortium. Data collection is projected to begin the fall of 2001, HAL willing.



Ben Craft (CAMD, LSU) and G. Balendiran (“Bali”) discuss design details of the MAD line being constructed in Baton Rouge.

Because of the mildness and beauty of the day, many were tempted to chat outside during the breaks. Inside, posters were on display and vendors’ booths (Molecular Structure Corp., Bruker, Blake Industries, and Oxford Scientific) demonstrated apparatus and systems.

One has to live in the southwest to have an appreciation for the distances (“mean-free-path”) separating groups and the consequent importance of such symposia to convey both the scientific and social aspects of our field, especially for students and post-docs, who are less likely to be able to travel to national and international meetings. These annual symposia have continued for a decade because they succeed at meeting a need. Out of them has come the user consortium which has established and will utilize a regional synchrotron beam line, so that productivity will continue to increase during the year, decade, and century to come.



Ken Usher (Dallas) describes to Keith Moffat the complications enfolded in the structure of Sap A, an Fe transport pore which consists of a large b-barrel and a long peptide terminus which sometimes? always?? blocks one end of the pore.

The tone set by the keynote speakers was a view of crystallography: past, present, and future. As we peer into the next decade, century, and millennium, those present could hear leading figures help celebrate both the accomplishments of our discipline but also challenge us for the years ahead.

Edgar Meyer

Pharmaceutical Powder X-Ray Diffraction Symposium, Newton Square, PA, September 27-30, 1999

The Pharmaceutical Powder X-Ray Diffraction (PPXRD) Symposium was held at the International Centre for Diffraction Data on September 27-30, 1999. There were approximately 95 participants from 9 different countries. The Symposium was divided into four main areas:

- Acquisition and Use of Powder Diffraction Data
- Polymorph Characterization by X-Ray Powder Diffraction
- Indexing, Structure Determination and Molecular Modeling
- Preformulation, Formulation, Regulatory and Patent Issues

The general results presented at the PPXRD showed the great utility of powder diffraction as finger prints. But moderate size unit cells and low symmetry conspire to produce a high density of Bragg peaks. Classification, quantification and isolating pure phases are made more difficult for pharmaceutical materials. Grinding samples to minimize preferred orientation can sometimes lead to stress-induced phase transitions; relative humidity control is often necessary. Data were presented on two polymorphs of terephthalic acid (TA-I and TA-II) for which the powder patterns were essentially indistinguishable. Polymorph discrimination is still extraordinarily difficult. In both R&D and process control, multi-probe techniques, e.g., DSC, TGA and XRD, are often required for sample analysis. In this case, one approach is to perform reaction pathway analyses that lead to the development of polymorph “roadmaps.” Controlled sample environments may be required and hydration/dehydration studies may be indicated.

A number of papers focussed on the use of direct methods and Monte Carlo simulated annealing techniques to perform structure determination. Fairly complex molecules, with 15-25 degrees of freedom have been solved. In these cases, torsion, translation and rotational degrees of freedom for the molecule are considered. Salts and solvates are more complicated, but still amenable to solution. The use of synchrotron sources to improve the pattern resolution, to adjust the scattering contrast, and improve the inherent signal to noise ratio are significant assets. Interestingly enough, one of the major areas for potential future development may be in the area of improving the reliability of techniques for indexing powder patterns. The burgeoning use of sophisticated structure determination tools will always be limited by the reliability of the indexing problem. Structure determination techniques on powders is still very much dependent on the starting assumptions concerning the chemical reasonableness of the molecular fragment.

John Faber

CSSP, Washington, D.C., December 4-6, 1999

The Council of Scientific Society Presidents (CSSP) consists of presidents, presidents-elect, and past presidents of about 60 physical, mathematical and life sciences, and science and math education organizations together with some academic and industry affiliate members which are usually represented by the vice presidents for research. About 115 people attended this meeting.

Saturday sessions were geared toward educating new members about research funding issues and ways of establishing communications with legislators. On the plane I had just read the *Science* article about the 15% increase in funding for NIH described as a “a last-minute minor miracle”. The budget plan would have required NIH to push 7.5 billion of their budget into FY2001, but lawmakers were persuaded to reduce the deferred amount to just 3 billion. Our first speaker, Mary Woolley, was the driving force behind this minor miracle. She told us that, unlike scientists, politicians usually give considerable credence to survey results. Surveys show that 66% of the general public supports doubling government spending on medical research in 5 years and that 81% believe that “Even if it brings no immediate benefits, basic research which advances the frontiers of knowledge is necessary and should be supported by the Federal Government.”

During the next two days, a number of general interest topics were discussed. I will mention only two. One is the recent decision by the Kansas Board of Education to eliminate evolution from the state science standards. John Staver, a member from

Kansas, told us that the group most threatening to evolution teaching is the “Intelligent Design” people (based in Seattle) because this group includes a number of scientists who, although not in the mainstream of science, do have credentials impressive to the general public. There is also a troubling Gallup poll indicating that 44% of Americans believe that “God created man pretty much in his present form at one time within the last 10,000 years,” a result that has remained stable for at least 15 years.

The other is the dismaying spectacle of the full-page ad (cost about \$60,000) in the Nov. 18th *Washington Post* requesting that Secretary Richard Riley withdraw his list of exemplary and promising mathematics programs, an event gleefully heralded by the press as the “Math Wars”. The objections, initiated by a small but vocal group of mathematicians, had been endorsed by a larger and more eminent group that apparently lacked much direct knowledge of the K-12 mathematics teaching curriculum. CSSP members expressed regret that this happened since confidence in these programs as models was undermined and models are urgently needed.

We heard sobering statistics about our probable future in the light of population increases and environmental/ecological trends described in a fascinating talk by Sandra Postel, Director of the Global Water Policy Project, Amherst, MA. Her research is clearly described in her books “Last Oasis” and “Pillar of Sand: Can the Irrigation Miracle Last?”.

Connie Chidester

Final FY 2000 Figures for the NSF

Following months of uncertainty about the FY 2000 appropriation for the National Science Foundation, there is positive news from Capitol Hill. The final bill contains a 6.5% increase in the total budget for the NSF. "It's a win for the economy and the nation," said NSF Director Rita Colwell.

"I can't believe it; I just can't believe it," is how Senator Barbara Mikulski (D-Maryland) put it at the end of the two hour conference committee on the bill. In one of the first instances of true cooperation between the administration and Congress in the final appropriations process, a way was found to add \$600 million to the amount available for the over-all bill. This helped to enable the following for the NSF in FY 2000:

Total NSF Budget: Up over this year by 6.5%, or \$238.8 million to \$3,910 million.

Research and Related Activities: Up 7.1%, or \$196.0 million to \$2,966.0 million.

Education and Human Resources: Up 5.3%, or \$35.0 million, to \$697 million.

Major Research Equipment: Up 5.6%, or \$5.0 million, to \$95 million.

How was all of this money found? Part of it came from unused housing funds, while other money was advanced from funding for FY 2001. NSF Director Colwell issued a statement praising House VA/HUD Appropriations Subcomm. Chair James Walsh (R-NY), Senate VA/HUD Appropriations Subcomm. Chair Christopher "Kit" Bond (R-Missouri), House VA/HUD Ranking Member Alan Mollohan (D-W VA), and Senate VA/HUD Ranking Member Barbara Mikulski (D-MD.) Colwell remarked that they and their fellow conferees "demonstrated extraordinary leadership and a clear understanding of the importance of investing in science and engineering."

Colwell also thanked other members of the House and Senate "who voiced their support for NSF during the appropriations process." They were Senate Majority Leader Trent Lott (R-Mississippi), Senate Appropriations Comm. Chair Ted Stevens (R-Alaska), Senate Appropriations Comm. Ranking Member Robert Byrd (D-W VA), House Science Comm. Chair James Sensenbrenner (R-WI), House Science Committee Ranking Member Ralph Hall (D-TX), House Basic Research Subcomm. Chair Nick Smith (R-MI), House Basic Research Subcomm. Ranking Member Eddie Bernice Johnson (D-TX), and Representative Vern Ehlers (R-MiI).

It would be hard to overstate the difficulty these and other members of the House and Senate leadership, and administration officials faced as they crafted the final figures in this bill. Reports indicate that OMB Director Jack Lew was instrumental in making this happen. Letters of acknowledgment of their efforts are in order. "The action by the conferees will enable scientists and engineers across the nation to do 21st century science," said Colwell.

FYI - AIP Bulletin of Science Policy News October 13, 1999, Richard M. Jones Public Information Division

Congress Finishes Work on Key Bills

Congress adjourned before Thanksgiving, and will not return to Washington until January 24. Adjournment was repeatedly postponed as several contentious issues, ranging from international family planning to dairy price supports, were either resolved or postponed (said House Majority Whip Tom DeLay (R-TX), "Exhaustion is your friend.") Before leaving town, they completed work on five appropriations bills and other legislation. Of note:

NIST: Any "fine print" concerning the FY 2000 appropriations is not yet available. (The five appropriations bills were combined into one bill of 2,000 pages, which is now being printed.) It is known that the Advanced Technology Program received \$130 million, a 27.0% cut. A White House summary stated, "While the House proposed eliminating the program, the final budget will allow ATP funding for an additional \$51 M in new awards." The NIST construction budget fared much better, almost doubling over FY 1999.

Math and Science Education: The Eisenhower Professional Development State Grants Program received \$335 million, the same as last year and as the original request.

Across the Board Cut in FY2000: The Republican congressional leadership pushed hard for an across-the board cut; the administration pushed hard against it. They compromised on a 0.38 percent cut in discretionary spending. Department and agency heads will be able to decide how to apply this cut within their overall budget, although no one program can be cut by more than 15%. An example of the impact of this cut is the National Science Foundation: its \$3,910M budget was reduced by \$14.858 million. Before this reduction, the total NSF budget was up 6.5%.

National Institutes of Health: The NIH budget rose by 15% to \$17.9 billion. To help balance the books, \$4 billion of this spending is delayed until September 29, 2000, pushing the cost into FY 2001. The original plan was to delay \$7.5 billion, which Health and Human Services Secretary Donna Shalala and medical researchers vigorously opposed.

R&E Tax Credit: After much negotiation between Congress and the Administration over how long this credit should be extended, a settlement was reached. In the words of the House Ways and Means Committee summary, the bill "Extends the research credit and includes an increase in the alternative incremental credit. Research credits attributable to the period after 6/30/99, and before 10/1/00, could not be taken into account by the taxpayer until 10/1/00. The expired provision generally provides for a 20% tax credit of qualified research expenditures. Extension: 5 years, through 6/30/04."

Employer-Provided Educational Assistance: Also in the tax bill was an extension for this exclusion. According to the Ways and Means Committee: "Extends the tax exclusion for employer-provided educational experience for undergraduate-level courses only. Generally, educational expenses paid by an employer for its employees are generally deductible by the employer. Extension: approximately 2.5 years, through 12/31/01."

FYI - AIP Bulletin of Science Policy News November 23, 1999, Richard M. Jones Public Information Division

New Definition of Research Misconduct

After four years of consideration, the Office of Science and Technology Policy (OSTP) and the National Science and Technology Council have drafted a single definition of research misconduct that will apply to all federally-sponsored research, along with uniform guidelines for conducting fair and timely investigations into allegations of misconduct. The proposal was published in the October 14 issue of the Federal Register. There was a 60-day period for public comment. At the end of this period, all feedback was to be reviewed and considered before issuance of a final policy to all federal agencies that support research.

Currently, many federal departments and agencies sponsor research, but not all use the same definition of misconduct, nor follow the same procedures when misconduct allegations have been made. The new policy was developed after extensive consultation with the primary federal R&D agencies, and builds upon their current policies. It will provide coherence across all federally-funded research, regardless of performer or location: research conducted at universities, private labs, federal intramural labs, and contractor-operated labs will all operate under the same misconduct guidelines.

Definition: Research misconduct, as defined in the proposal, comprises “fabrication, falsification, or plagiarism in proposing, performing, or reviewing research, or in reporting research results.” Each of these terms is then defined in more detail. It is noted that “research misconduct does not include honest error or honest differences of opinion.”

Procedures: According to the proposal, a finding of research misconduct requires that “there be a significant departure from accepted practices of the scientific community for maintaining the integrity of the research record; the misconduct be committed intentionally, or knowingly, or in reckless disregard of accepted practices; and the allegation be proven by a preponderance of evidence. The notice then describes “Responsibilities of Federal Agencies and Research Institutions” upon an allegation of misconduct, including phases of the investigation and what

aspects are to be handled by the federal agency versus the home research institution. “Guidelines for Fair and Timely Procedures” include safeguards for informants and the subject of the allegation, objectivity and expertise, timeliness, and confidentiality. Finally, in the case of a finding of misconduct, the appropriate administrative actions are discussed.

Supplementary Information The notice also includes several paragraphs of Supplementary Information, of which a portion is quoted here: “The proposed policy defines the scope of the Federal government’s interest in the accuracy and reliability of the research record and the processes involved in its development. It consists of a definition of research misconduct and establishes basic guidelines for responding to allegations of research misconduct, including procedural safeguards. An important objective of this policy is to achieve uniformity across the Federal agencies in the definition of research misconduct they use and consistency in their processes for responding to allegations.... The proposed policy addresses behavior subject to administrative action and applies only to research misconduct as defined in the policy. It does not supersede government policies or procedures for addressing other matters, such as the unethical treatment of human research subjects or mistreatment of laboratory animals used in research, nor does it supersede criminal or civil law. It does not limit agency or institutional policies and prerogatives in addressing other forms of misconduct, including those that might occur in the course of conducting research, including the misuse of public funds.”

To Read the Entire Notice: The Table of Contents for the October 14, 1999 issue of the Federal Register can be found at the following web site: http://www.access.gpo.gov/su_docs/fedreg/a991014c.html This notice is found near the very bottom of the Table of Contents, under “Science and Technology Policy Office, Notices.”

FYI - The American Institute of Physics Bulletin of Science Policy News October 19, 1999. Audrey T. Leath Public Information Division The American Institute of Physics - fyi@aip.org - <http://www.aip.org/enews/fyi/>

Denver X-ray Conference

The 2000 Denver X-Ray Conference, sponsored by the International Centre for Diffraction Data, will be held July 31 – August 4, 2000 at the Denver Marriott Tech Center Hotel in Denver, CO.

The *plenary session* will cover X-ray Analysis in the 21st Century. There will be *special sessions* on: Major Problems in XRD & XRF and Possible Solutions; Microbeam Techniques; Phase Transformation; Mesostructure Analysis; New Developments in XRD Instrumentation; XRD in Pharmaceuticals; Thin Films Analysis; Residual Stress Computational Design; New Developments in XRF; TXRF; XRF in Metal and Mining Industries; XRF in Petroleum Exploration; Thin Films Analysis XRF; Quantitative & Software.

Workshops will include: New Methods of Beam Conditioning; Phase Transformation; Analysis of Micron Size Specimens; Grazing Incidence; Hands on Rietveld Analysis; Residual Stress Analysis; Texture Analysis; Alignment & Standards; Specimen Preparation XRF; Practical TXRF; Fundamental Parameters; Introduction to XRF

For details check the Conference Website: <http://www.dxcicdd.com/>

Year 2000 ICDD Clinics on X-ray Fluorescence Spectrometry and X-ray Powder Diffraction

Fundamentals of Fluorescence Spectrometry, May 1-5

Covering basics of X-ray spectra, instrumentation design, methods of qualitative and quantitative analysis, specimen preparation and applications for both wavelength and energy dispersive spectrometry.

Advanced Methods in Fluorescence Spectrometry, May 8-12

Emphasizing quantitative methods, use of automated X-ray spectrometers, review of mathematical matrix correction procedures, and new developments in XRF.

Fundamentals of Powder Diffraction, June 5-9

Covering instrumentation, specimen preparation, data acquisition, and qualitative phase analysis.

Advanced Methods in Powder Diffraction, June 12-16

Emphasizing computer-based methods of data collection and interpretation, both for qualitative and quantitative phase analysis.

For further information, please contact:

Jeanne Ginsburg at clinics@icdd.com

Web-site: <http://www.icdd.com/education/clinics.htm>

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7. I certify that the statements made by me above are correct and complete. (Signed) Marcia Colquhoun for American Crystallographic Assn.

SAS Workshop, Univ. of Georgia, April 7, 2000

The workshop will cover the use of single wavelength anomalous scattering data in phasing macromolecular structures; applications to both in-house and synchrotron data. The morning session will discuss theory and application; the afternoon session will be hands-on demonstrations and structure determinations. Feel free to bring and work on your own data. Enrollment limited to 30. Organized by Bi-Cheng Wang. For more detail, see <http://www.uga.edu/~biocryst/sas00/>

Rietveld Method Short Course, Georgia Tech, Atlanta GA, May 8-10, 2000

The Rietveld method is widely recognized to be uniquely valuable for structural analysis of nearly all crystal structure and related analyses for materials not available as single crystals. This 3-day intensive course will be conducted by Professors Angus P. Wilkinson, R.B. Von Dreele, and R.A. Young. The course will deal with the principles and techniques of Rietveld analysis and with avoiding or overcoming problems encountered in the use of it. The teaching system involves morning lectures, supervised individual hands-on experience running the Rietveld refinements on PC-type computers in the afternoon, much student-teacher interaction and discussion, and availability of the computers at other times for further individual practice. The student will have a choice of using either of the two most widely used Rietveld programs, DBWS and GSAS. Both the well grounded beginner and the moderately experienced user should find the course valuable.

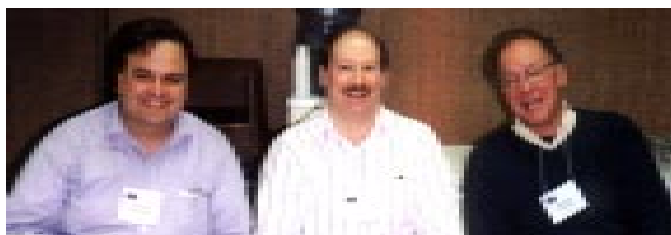
The course is conducted by Georgia Tech Continuing Education and costs \$995 (includes monograph and copies of computer programs and examples). For more information: Contact Continuing Education, Georgia Institute of Technology, Atlanta, Georgia 30332, Ph: (404)-385-3502, e-mail: angela.arnold@conted.gatech.edu, Web: www.conted.gatech.edu

Centrifugal Materials Processing IV, May 29 to June 2, 2000

The Fourth International Workshop on Materials Processing at High Gravity will be held at Clarkson Uni., Potsdam, New York 13699-5814. Contact: Prof. Liya L. Regel, <http://www.clarkson.edu/~regel/workshop.htm> or regel@clarkson.edu Ph: (315) 268-7672 Fax: (315) 268-3833

ACA Summer Schol 2000, University of Georgia, July 7-19, 2000

Contact: B.-C. Wang (phone 706-542-1747) or John Rose (phone 706-542-1750), Department of Biochemistry, University of Georgia, Athens, GA 30602 - <http://BCL5.bmb.uga.edu/aca2k.html>

ACA 2000, St. Paul, MN, July 22-27, 2000

Program Chair: Doug Ohlendorf (UMN), Local Chairs: Victor Young (UMN) and Bill Gleason (UMN)

25-31 19th European Crystallographic Meeting ECM 19, Nancy, France, August 25-31, 2000 -

Chair: Claude Lecomte. e-mail: ecm19@lcm3b.u-nancy.fr. URL: www.lcm3b.u-nancy.fr/ecm19/.

International Workshop on Physical Characterization of Pharmaceutical Solids, September 24-29, 2000.

The workshop, held in cooperation with Cambridge Crystallographic Data Centre and Glaxo Wellcome, will take place in Lancaster, Pennsylvania. It is of particular interest to scientists working in the areas of drug discovery, preformulation, formulation, stability testing, and product development. For further information please contact J. Matthew Grant, Advanced Solid State Characterization, Inc., Tel: (610) 594-2081, Fax: (610) 594-2082 Web Site: <http://www.assci.com/~marekz/IWPCPS-1.htm>

ACA 2001, Los Angeles, CA, July 21-26, 20001

Program Chair: Duncan McRee (Scripps), Local Chairs: Dan Anderson (UCLA) and Katherine Kantardjieff (CSU-Fullerton).

ACA 2002, San Antonio, TX, May 25-30, 2002: Local Chairs: Ray Davis (UT Austin) and Marv Hackert (UT Austin).

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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/>

New Positions

Postdoctoral Fellow

The objective of our program is to determine the atomic structures of key proteins in the muscle machine in different physiological states. Our goals are to understand the molecular basis of motor activity in the myosin molecule and its calcium control by the troponin/tropomyosin complex bound to actin. Strong collaborative support is available in the molecular biology and biochemistry of these systems. This research effort is one of a number of programs in the Structural Biology Laboratory at Brandeis which has excellent facilities and state of the art equipment for a broad range of studies.

Interested candidates with a good background in protein crystallography should send a letter and CV, together with names, addresses and telephone numbers of three scientists from whom letters of recommendation can be obtained, to: Dr. Carolyn Cohen, Rosenstiel Basic Medical Sciences Research Center, Brandeis University, Waltham, MA 02454-9110, E-mail: ccohen@binah.cc.brandeis.edu, Phone : 781-736-2446, FAX: 781-736-2405

Research Scientist

Agouron Pharmaceuticals Inc., a leader in the use of X-ray structure analysis for the design of small molecule drugs, has an opening for a highly motivated technical scientist to join its protein crystallography group. Applicants should have a B.S. or M.S. degree in biochemistry or a related discipline with experience in protein purification and crystallization. The successful candidate will work in a challenging, exciting research environment as part of an interdisciplinary drug discovery team and will be responsible for crystallization of biological macromolecules and their complexes with selected ligands. We offer competitive salaries and benefits in a superb location. For consideration please send cv to Human Resources Department,

Job Code 110-DM, Agouron Pharmaceuticals Inc., 10777 Science Center Dr., San Diego, CA 92121. Application materials can also be sent to the attention of Job Code 110-DM

Positions Previously Listed

Postdoctoral Positions

Enzyme Crystallography, Mechanisms, Molecular Biology. Send your curriculum vitae to Dr. William Lipscomb, Department of Chemistry and Chemical Biology, 12 Oxford St., Cambridge, MA 02138. Lipscomb@chemistry.harvard.edu, FAX: (617) 495-3330.

A postdoctoral position is available in the laboratory of Michael Rossmann for a person with interest in computational macromolecular crystallography. The research will be primarily in developing improved, three-dimensional, methods for the analysis of single crystal X-ray diffraction data of proteins, viruses, nucleic acids, and other large biological complexes. Emphasis will be on data collected at synchrotrons. Previous experience in the development of computational crystallographic techniques and of common computer languages is essential.

Please send applications including a CV and the names of three referees to Michael Rossmann, Hanley Professor of Biological Sciences, Department of Biological Sciences, Purdue University, West Lafayette, Indiana, 47907-1392, USA. Email address: mgr@indiana.bio.purdue.edu. Phone number: 765-494-4911. Fax number: 765-496-1189.

Research Specialist

The Howard Hughes Medical Institute, a leading biomedical research organization, located at the University of Texas Southwestern Medical Center in Dallas, TX, is currently seeking a Research Specialist. This position will manage and maintain a protein X-ray diffraction facility for the structural biology group including rotating anode X-ray generators, image plate detectors, liquid nitrogen cryo systems and associated computing hardware and software. Candidate must have 2 years experience and a background in electronics, precision machining skills and familiarity with the UNIX operating systems. HHMI offers a competitive salary and benefits package. To apply, send resume and salary history, with three complete references, to: HHMI, Attn: HR-SPG, 5323 Harry Hines Blvd., Y4.226, Dallas, TX 75235-9050. Fax: (214) 648-5066. E-mail: davist@hhmi.org. HHMI is an equal opportunity employer.