

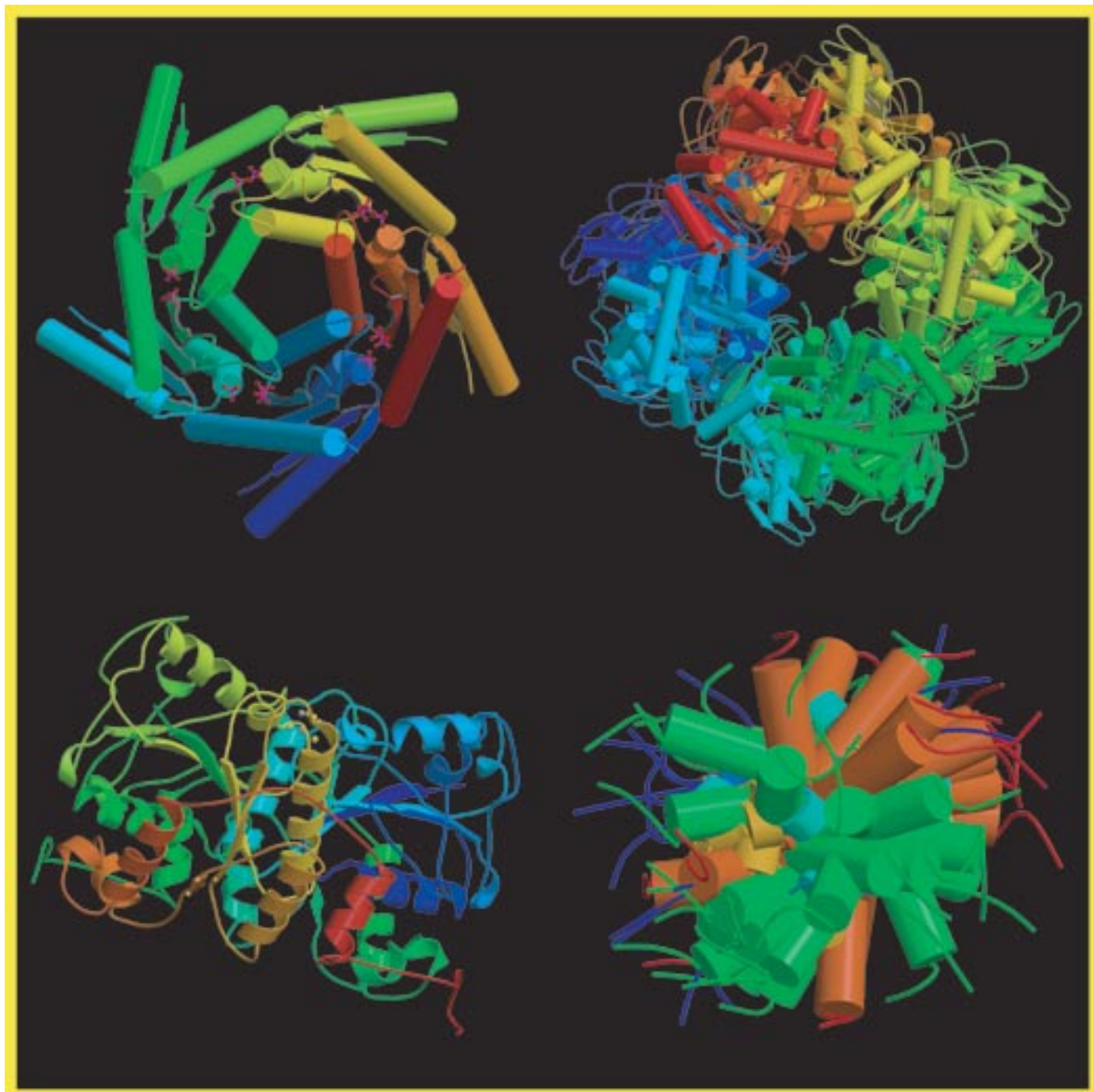


AMERICAN CRYSTALLOGRAPHIC
ASSOCIATION

NEWSLETTER

Number 2

Summer 2002



The Art of Science

Images from the Protein Data Bank

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President's Column



The San Antonio meeting was successful in nearly every sense of the word. For an IUCr year, the attendance of ~730 participants, plus 75 corporate registrations was well above expectations. The local committee worked with precision teamwork, and the scientific program elicited well-deserved compliments from every sector of the membership. Symposia

on electron diffraction crystallography and electron microscopy occasioned by the Patterson award to Doug Dorset drew new faces to the meeting. The ACA Transactions Symposium on powder diffraction, organized by Abe Clearfield, was also very well-received. Abe was able to set a standard for publication of this event by collecting manuscripts for nearly all of the presentations, and we can gratefully expect timely publication! These symposia highlighted the multidisciplinary ACA mission to support all investigations into the structure of matter. The electron microscopists and powder diffractionists are mounting efforts to found new ACA SIGs .

The Institute of Texan Cultures museum provided a splendid venue for the Awards banquet. ACA Past-President Bill Stallings recalled the first meetings of American crystallographers at Gibson Island Maryland in 1941, reminding us of a time when a five-day program had only one set of nine speakers that, even then, included macromolecular crystallography. Afternoons were free for swimming, boating and golf. It was humbling to note that one of the highest-powered scientific figures of that time (Lindo Patterson) did part of the the organizational work. Bill also documented an interesting connection between these meetings and the Gordon Conferences. Wood Scientific Writing Award winner Ira Flatow regaled us with a spirited description of the role of experimentation in developing his inimitable journalistic style. Heartfelt thanks to ACA Vice-President Ray Davis and USNCCr Chairman Marv Hackert for taking time off from these duties to make such flawless local arrangements!

During the course of the week, the ACA Council advanced many fronts of interest to the membership. The Margaret Etter Early Career and Lectureship Awards were distinguished from one another. Both arise from the fund established in memory of Peggy Etter and will be used specifically to recognize and encourage young crystallographers. The former will recognize one crystallographer annually during the first six years of an independent career. The latter is a smaller award that will be given to one student from each SIG whose work is selected from the contributed abstracts for an oral presentation. Nominations for the Early Career Award will be sought from SIGS, as well as from departments that hire crystallographers.

We were very happy to welcome scientific contributions from ~15 Latin American scientists. Council met with them to explore ways that the ACA, as IUCr regional affiliate for the western

hemisphere, could help strengthen crystallography throughout their region. Such efforts will depend on enhancing two-way scientific exchange programs that encourage growth of personal contacts between laboratories in the region. Equally important seems to be a stronger sense of participation by the Latin American crystallographers in intra and inter-regional affiliations. To that end, signatures are being solicited from current ACA members in Latin America to form a new SIG to interface with Council on all relevant matters. Council also decided to start a new fund whose assets will help advance this initiative, including provision of partial support for our Latin American colleagues to attend ACA meetings. I call your attention to this new fund, and encourage you to contribute generously. ACA Executive Officer Bill Duax has provided the new fund a running start by offering to match the first \$1000 in donations.

The ACA education mission was a major focus of Council deliberations, due in part to the need to pass the torch for the ACA Summer School from the Univ. of Georgia, and B. C. Wang in particular, to new stewards. Five proposals were submitted to council underscoring the need for such courses. Available courses are oversubscribed, and there is the perennial concern that the explosive growth of crystallography in service to other disciplines creates a continuing need for fundamental training. As none of the five proposals offered a complete replacement to the former course, we decided on an interim solution. In 2003 the ACA will support a modest course in small molecule fundamentals at Indiana Univ. of Pennsylvania, and a more extensive course, primarily centered on macromolecular crystallography, at the Illinois Institute of Technology in Chicago.

These courses may not fully satisfy the needs of the community. Crystallography occupies a unique position among scientific disciplines, providing vital data used in developing physics,

chemistry, biology, and geology, but having for this reason, no independent representation either in most university curricula or on any federal funding agency. Balanced against this decentralization is the obvious vitality of teaching efforts within the community itself, as evidenced by the five competing proposals for the summer school. Clearly it is desirable to foster more teaching of young crystallographers. With the ACA budget roughly stable, or perhaps declining slightly, this effort cannot be mounted without securing other support. One possibility is to seek scholarship support on a continuing basis from federal agencies, and this has become a priority.

I opened this letter saying that the San Antonio meeting was "nearly" perfect. Unfortunately, something happened there that distressed me deeply. We have become accustomed to important scientific presentations being restricted by proprietary interests that have, to date, resulted in only modest suppression of discussion. However, in San Antonio, the recent explosive growth of corporate crystallography produced its first real challenge to our scientific and intellectual health. Industry-based speakers invited to discuss their work were replaced by "company" personnel because the invited speakers were no longer associated with a particular company. For the first time in my experience both platform and informal discussions were compromised by constraints arising from real and threatened hostile legal action based on what many found to be a miscarriage of patent law. While admitting that much remains to be learned, these examples represent new and highly unwelcome pathologies that threaten to disrupt broad aspects of scientific exchange. I personally hope that such "automatic" reassignment of platform speakers will be strongly discouraged and that the legal adventurism will fail. It is essential that we minimize the very real threat of intellectual nuclear winter.

Charlie Carter



New Awards honoring the late Professor Peggy Etter

In recent years the ACA has selected one or two students for special recognition by means of a special travel award named after the late Professor Peggy Etter. This has been an *ad hoc* arrangement that has operated alongside the Student Travel Awards that assist many students from North America and overseas in attending ACA meetings to present their work.

At the most recent ACA Council Meeting on May 24th, 2002 in San Antonio, a decision was taken to formally implement *two* separate awards named after Peggy Etter. These awards not only recognize Professor Etter's tremendous scientific accomplishments but also her well-deserved reputation as an outstanding mentor of students and junior colleagues alike. The **Margaret C. Etter Early Career Award** will recognize achievement and future potential among those at an early stage in their independent career. The citation for the award and the guidelines for submitting nominations are given below. The **Margaret C. Etter Student Lecturer Award** will be presented to a small group of students each year who have been selected to give oral presentations at the ACA meeting. The award will be entirely independent of the ACA travel awards, which will remain open to students, postdoctorals and young scientists.

Nominations for the Early Career Award may come from any source, but the SIGs have been encouraged to take an active role in identifying candidates for this award from their area of expertise. Thus, the SIG guidelines will be modified to include this activity as well as the responsibility for selecting winners of the Student Lecturer Award.

Margaret C. Etter Early Career Award. To recognize outstanding achievement and exceptional potential in crystallographic research demonstrated by a scientist at an early stage of their independent career. The award is established to honor the memory of Professor Margaret C. Etter (1943-1992), who was a major contributor to the field of organic solid-state chemistry. Her work particularly emphasized the use of hydrogen bonds and co-crystals. In addition to a large body of experimental work she was the major force in devising a set of rules known as graph sets to describe hydrogen bonds in a way that revealed similarities between structures without being tied up in the crystallographic details. Her experience teaching at an undergraduate institution and in working in both an industrial and academic setting gave her an unusually broad perspective from which to mentor students and to support and encourage colleagues. She had a love for people, for science, and especially for people who do science, that we honor. Established in 2002 as an annual award, it consists of an honorarium plus travel expenses to accept the award and present a lecture at the American Crystallographic Association annual meeting.

Award Guidelines

Scientists involved in crystallographic research in the broadest sense will be eligible for the award. At the time of the closing date for nominations, nominees must be no more than 10 years beyond the awarding of their Ph.D. degree, not including

career breaks, and must have begun their first independent (not postdoctoral) position within the past 6 years. Nominees employed in tenure-track academic positions must not yet have received tenure.

Nominations must include as a minimum a nomination letter clearly indicating the accomplishments of the individual since beginning their independent career and assessing the future potential of the nominee. Additional supporting letters and a c.v. for the nominee may be provided but are not requirements. Self-nominations are not permitted.

Nominees may be employed in regular academic positions, as service crystallographers, in industrial positions or in government laboratory positions.

The closing date for nominations will be September 1st directly prior to the ACA meeting at which the award will be presented. The nominations will be evaluated by the ACA Council at their Fall meeting.

Nominations should be postmarked before the closing date and submitted to:

Margaret C. Etter Early Career Award
American Crystallographic Association
P.O. Box 96 Ellicott Station
Buffalo, NY 14205-0096

Margaret C. Etter Student Lecturer Award. Each Special Interest Group (SIG) within the ACA has the opportunity to select *one* student to receive an award and to present a lecture in one of the sessions organized by that SIG. Selections are based upon submitted abstracts and are independent of whether the student presenter originally requested an oral or poster presentation. Award winners are determined by the elected officers of the SIGs. Students who are selected receive a monetary award of \$250, which is independent of any requests for support via the ACA Travel Awards.

The abstract submission forms will be modified to include a check-off box to identify student presenters.

Lee Brammer, Secretary



*"Glide planes"
from Wally Cordes'
ACA poster on
teaching crystallo-
graphy*

ACA announces 2003 winners of Warren and Buerger Awards and 2002 selectee for ACA Service Award

During the ACA meeting in San Antonio, the award committees for the Buerger and Warren Awards announced the winners of the 2003 awards.

The selection committee (Paul Butler, chair, Jacqueline Johnson, Ian Robinson, and Boguslaw Stec) is pleased to announce that in 2003 the **Bertram E. Warren Diffraction Physics Award** will be presented to **James Ibers** of Northwestern University.

The selection committee (James Kaduk, chair, Robert Blessing, Gerard Bricogne and Sylvie Doubleie) is pleased to announce that in 2003 the **Martin J. Buerger Award** will be presented to **Takeshi Egami** of the University of Pennsylvania.

The awards will be presented at the ACA meeting in greater Cincinnati (Northern Kentucky) in July 2003. Symposia will be planned around the winners of the two awards. This practice follows from the highly successful awards symposium associated with presentation of the **Patterson Award** to **Doug Dorset** at the San Antonio meeting. Further details of the award winners and the official award citations will be published in the fall *Newsletter*.

Lee Brammer

S. N. Rao named as the 2002 selectee for the ACA Service Award.



The Award, presented at the banquet in San Antonio, was presented to Dr. Rao for his long and dedicated service to the ACA as treasurer, financial officer and official negotiator for ACA meeting contracts.

At the banquet in the Institute of Texan Cultures



Patterson Award winner Doug Dorset (center) with Chris Gilmore (left) and Walter Pangborn (right)



Bernie Santarsiero and Tom Koetzle discussing science with an unidentified crystallographer

Wally Cordes
Vice President



University Professor, Department of Chemistry and Biochemistry, University of Arkansas, Fayetteville, Arkansas, 72701.

Education: B.S. in Chemistry, Northern Illinois University, 1956; Ph.D. in Inorganic Chemistry, University of Illinois, 1960. My initial crystallographic education was at Cal Tech (1966 sabbatical with Dick Marsh, Jurg Waser, Sten Samson, and Bill Schaefer), followed by subsequent sabbaticals with Larry Dahl, Jim Trotter, and Peter White. I now receive continuing education from my former students, especially B.C. Wang, Paul Swepston, and Bill Pennington.

Professional Activities: ACA: In the past: chairman of the Small Molecule SIG and member of the Continuing Education Committee. Currently: program co-chair (with Travis Gallagher) for the San Antonio annual meeting. Instructor at the ACA Summer School in Crystallography for four years. Other: Editorial Board for Journal of Chemical Crystallography, reviewer for a variety of journals, chairman of the Chemistry Department at the University of Arkansas, 1984-7.

Research Interests: Small molecule crystallography, structures of main-group inorganic ring and cluster molecules, structures of S-N and organic radical materials which are molecular metals (collaborations with Richard Oakley and Robert Haddon). Crystallographic Education.

Statement: Like most ACA members, I've never met a crystal that I didn't like. It is hard to think of an activity that is more satisfying and more fun than structural research. It is always a thrill to see those first reflections from a new crystal: in early days that happened when one pulled the first films out of the developer solution. Following that were years of hearing the first squeal of a CAD-4 speaker connected to the detector circuit, and now it is seeing spots on a monitor as the first image is displayed. Those first reflections are exciting, as is seeing the first atoms of a never-before-seen structure. If chemistry is the "Central Science", as the textbooks proclaim, then certainly structural research is the "Central Experiment" (often the "method of ultimate truth").

The ACA is a well-organized association. My current stint as a program chairman for the 2002 meeting makes it very clear how much the success of our meetings depends on a tremendous amount of labor and time put in by a large number of people — the SIG leaders and session organizers. Fortunately our organizational structure is excellent and up to the task. In this sense the ACA does not need new leadership to completely revamp the organization or to lead us into radically new directions, but more to be sure to keep our fine machinery running smoothly.

It is obvious from the contents of the programs of our annual meetings that the diversity of the structural research being done by our membership is expanding rapidly. Yet it is also apparent that there are overlaps in components of these different kinds of structural research, and one value of our organization is to bring these folks together so the synergistic effect can take place. It also means the ACA Council, in its important advocacy role for structural research in general, has to be ready to advocate in a very wide variety of arenas.

A concern expressed repeatedly in recent years is about crystallographic education — the amount of coursework offered in graduate programs is declining because many tenure-track "crystallographer-faculty" are retiring and not always being replaced. The ACA has a responsibility

here — and has addressed this responsibility with the Crystallographic Summer School. The continually-increasing numbers of applicants for student positions in that summer school, from its beginnings at Pittsburgh through its recent years at the University of Georgia, show the need. Finding a new home for that summer school, and providing support at our annual meetings for those who teach crystallography, should be on the ACA's "to-do" list.

ACA meetings are terrific: they demonstrate that crystallographers are friendly and helpful by nature. The number of members who return year after year is a testimony to the value of the meetings. We all go home with new ideas of strategies to apply to a research problem, and we also go home feeling we are well-informed on the rapidly changing hardware and software related to our research. One of the important responsibilities of the ACA Council is to maintain the vigor and the spirit of the annual meetings.

The ACA has been a key component of my career, and it is an honor to be nominated for this office. Independent of the outcome of the election, I hope I can continue to serve the ACA in some way as a repayment for all of the benefits I have realized from my association with this family.

Frances Jurnak
Vice President



Professor of Physiology and Biophysics, College of Medicine, University of California, Irvine, Irvine, CA 92697-4560

Education: B. S., Chemistry, Cath-

olic University (1968); Ph.D., Chemistry, University of California at Berkeley (1973). Mentors: Kenneth Raymond and David Templeton, UCB (Ph.D.); Alexander Rich, Massachusetts Institute of Technology and Alexander McPherson, Pennsylvania State University at Hershey (Postdoctoral, 1974-1979).

Professional activities: Co-director of Structural Molecular Biology Program, Chao Family Comprehensive Cancer Center, University of California Irvine (2000-2005); editorial board of *Journal of Structural Biology* (1997-2003); BCB study section member (1993-1996); *ad hoc* member of review panels for NIH and NSF; symposium organizer, American Society for Biochemistry and Molecular Biology, Atlanta, Georgia (1991); Co-Organizer of West Coast Protein Crystallography Workshop, Asilomar (1988); Dupont Lecturer, UC Berkeley (1995); Rosetta Briegel Barton Lecturer, University of Oklahoma (1991); Alberta Heritage Speaker, University of Alberta (1989).

Research interests: The laboratory studies the structures of important proteins in order to determine how the proteins function at the atomic level. One longstanding research problem is elongation factor, EF-Tu and its role in ribosomal protein synthesis. With the structures of the four cytoplasmic EF-Tu complexes now solved, efforts are focussed on EF-Tu-antibiotic complexes as well as on understanding EF-Tu's role as a chaperone and disulfide isomerase under conditions of cellular stress. Another research area involves pectate lyases and their structural homologues in plants. All share a parallel β helix topology and the same key residues in the active site, whether the protein functions as hydrolase, lyase, or both. Recently, the lab is shifting its structural focus toward proteins involved in carcinogenic mechanisms to use as targets for rational drug design studies.

Statement: It is a great privilege to stand for election as Vice-President of the American Crystallographic Association. The ACA has been instrumental in helping many crystallographers throughout their careers, including mine – from giving me encouragement as a younger researcher to being a home away from home and

meeting with colleagues who have become good friends over the years. The ACA has been a champion of crystallographic research, keeping its roots in x-ray diffraction techniques and small molecule research, while expanding into macromolecular crystallography as the field has grown to the wider horizon of structural genomics. As different research areas evolve and, in many ways, become more automatic, it is the ACA members that preserve the knowledge base necessary to achieve the next developmental level as newer technologies become available. Were I to be elected, I would serve in the same manner as I run my research program, conscientiously, with attention to detail and respect for all opinions, and always on the lookout for the latest scientific advances to enhance the research. In terms of an organization, this translates into attention for prominent scholastic issues, increasing membership and meeting attendance through quality programs, and passing the torch to the younger generation.

Lisa J. Keefe Secretary



User Program Coordinator, Senior Research Associate, Industrial Macromolecular Crystallography Association Collaborative Access Team (IMCAT), Illinois Institute of Technology at the Advanced Photon Source, Argonne National Laboratory, Argonne, IL 60439

Education: A.B. in Chemistry (1983) Vassar College; Ph.D. in Biophysics and Biophysical Chemistry (1992) The Johns

Hopkins University School of Medicine; DOE Alexander Hollaender Distinguished Postdoctoral Fellow (1992-96) at the Structural Biology Center, Argonne National Laboratory and Brookhaven National Laboratory.

Professional Activities: member of American Crystallographic Association; Steering Committee member of Advanced Photon Source Users Organization (APSUO); chair (1993-1994) of ACA Young Scientist Special Interest Group.

Research Interests: macromolecular crystallography; molecular recognition; cryocrystallography; automation and robotics; anomalous dispersion; synchrotron radiation

Statement: The office of secretary is delineated in the ACA constitution by two essential roles: administrative and serving as member of the ACA council. In the administrative capacity, responsibilities include recording meeting minutes, tending to correspondence, and maintaining a dossier of precedents and procedures. As council member, responsibilities include contributing to the general direction and management of the affairs of the ACA. Since I first joined the ACA, the growth in membership has been tremendous and stands as a testament to the strength of the organization and to the enormous benefit it offers its members. The opportunity to potentially serve in the capacity of secretary to the ACA and its membership is both a pleasure and an honor.

As secretary, I will commit the time and effort needed to maintain complete records of the meetings and to effectively communicate with the membership. My activities within the ACA have traversed both the scientific and organizational realms: participating in scientific presentations at meetings and serving as the first chair of the Young Scientist Special Interest Group (YSSIG). Thus, I have a realistic appreciation for the level of commitment required to successfully meet the demands of this office.

As a member of council, I will be committed to supporting all areas of crystallography and to representing the diversity of crystallographic disciplines. My crystallographic education began in

small molecule crystallography, extended to macromolecular crystallography, and broadened to include synchrotron radiation. My experience in working with many researchers at synchrotron user facilities has helped me understand the variety of needs, issues, and concerns of the crystallographic community. I have developed a broad perspective regarding the endeavors on which the ACA can focus in order to best serve its constituency.

I enthusiastically welcome the opportunity to serve the ACA and its membership.

Patrick J. Loll Secretary



Associate Professor of Biochemistry, MCP Hahnemann Univ., Philadelphia, PA,

Education: B. Ch. E. Chemical Engineering, Catholic University of America (1981); Ph. D., Biophysics, Johns Hopkins University (1989); Post-doctoral, University of Chicago (1989-1995).

Professional Activities: Reviewer for *Acta Cryst.*, *Arch. Biochem Biophys.*, *J. Am. Chem. Soc.*, *J. Biol. Chem.*, *J. Pharm. Exp. Therap.*, and *Proteins*; Member Biosciences Proposal Study Panel, Advanced Light Source; Review panels for NASA and NSF; ACA Pauling Prize committee (1998, 2002); Member,

Protein Society, Biophysical Society, and ACA (since 1988).

Research Interests: Membrane protein structural biology; macromolecular crystallization; structural basis of antibiotic activity; structure-based drug design.

Statement: The Secretary of the ACA performs administrative tasks that serve the organization. The ACA has been a valuable resource for me over the years, and I would be delighted to contribute to its continued success by discharging the duties of the Secretary. However, in addition to acting as the keeper of the organizational record, the Secretary is a member of the ACA Council, and as such has the opportunity to influence the future direction of the organization. I have two qualifications which I believe prepare me for this role: First, I have been exposed to many different aspects of crystallography, and these experiences have engendered in me an appreciation for the extraordinary diversity and scope of the discipline. Second, I possess the firm conviction that structural studies, and particularly those based on diffraction methods, lie at the heart of modern physical and biological science.

My research effort has always been centered around protein crystallography, which places me in the mainstream of the burgeoning structural biology "wing" of the ACA. This makes me keenly aware of the impending explosion of macromolecular structural data. These data will create unprecedented opportunities in crystallography. They will also pose tremendous new challenges that will force us to rethink the role of the crystallographer in this post-genomic world. In addition to having strong roots in structural biology, I am fortunate in that my scientific travels have exposed me to other areas of interest to the ACA, including chemical crystallography, methods development, solution scattering, and the teaching of crystallography to both crystallographers and non-crystallographers. These experiences have instilled in me a great respect for all things crystallographic. I believe it is critical that the ACA continue to represent the broadest possible spectrum of interests, and as your Secretary I would work diligently to make it so.

Louis T. J. Delbaere Communications Committee



Canada Research Chair in Structural Biochemistry, Professor and Head of Biochemistry, Univ. of Saskatchewan, Saskatoon, Saskatchewan, S7N 5E5, Canada

Education: B. Sc. Chemistry, University of Manitoba (1965), Ph. D. Chemistry, University of Manitoba (1970). PDF University of Oxford (1969-71), PDF University of Alberta (1971-73).

Professional Activities: ACA Council Canadian Representative, 1999-2001; Member IUCr Commission on Synchrotron Radiation, 1999-2002; Member IUCr Commission on Union Calendar, 1999-2002; Chair Working Group on Protein Crystallography Beamlines at the Canadian Light Source, 1999-2002; Chair Phosphotransfer Session International School of Crystallography Molecular Biology Erice Sicily, 2000; Canadian Delegate IUCr Congress and General Assembly Glasgow (Scotland), 1999; Program Chair ACA Annual Meeting Arlington (Virginia), 1998; Canadian Institutes of Health Research University Delegate, 1997-2002; Member National Cancer Institute of Canada grants panel, 2001-2002; Medical Research Council of Canada grants panel, Member 1991-93, 1999 and Chair, 1994-96.

Research Interests: Crystallographic studies of phosphoenolpyruvate carboxykinase to examine the active site residues and the mechanism of catalysis. Additional projects concern the structure and function studies of other important enzymes. This research involves the use of synchrotron radiation, so extensive use

will be made of the on-site Canadian Light Source after the facility is functioning in early 2004.

Statement: To be nominated for this Committee is an honor. For four years I was directly involved with ACA Council, first of all as Program Chair of the Annual Meeting in Arlington, Virginia and subsequently as the Canadian Representative on Council.

Communication among fellow scientists as well as between scientists and the general public and politicians is very important and the ACA should play an effective role in this matter.

The ACA produces high quality publications and we should strive to maintain this distinction. If elected I would do my best to fulfill the duties of this Committee.

Fusen Han **Communications Committee**



Senior Scientist, †“Structure, Analytical Medicinal Chemistry”, Pharmacia Corp., Kalamazoo, Michigan.

Education: BS in Physics, Chinese University of Science and Technology (1970). Ph.D., Crystallography, Chinese Academy of Sciences (1983). Postdoctoral fellow at Hauptman-Woodward Medical Research Institute (1986-1988).

Professional Activities: ACA member since 1985.

Research Interests: Small molecular crystal structures, methods development and computer programming.

Candidates for ACA offices in 2003

The Nominating Committee has selected the following candidates for the 2002 elections for ACA offices in 2003.

Vice-President: **Wally Cordes & Frances Jurnak**

Secretary: **Lisa Keefe & Patrick Loll**

Committees:

Communications: **Louis Delbaere & Fusen Han**

Continuing Education: **Andy Howard & Kathy Kantardjieff**

Data Standards & Computing: **Steve Muchmore & Bob Sweet**

2002 Nominating Committee:

Tom Terwilliger (Chair), Connie Chidester and Winnie Wong-Ng

To nominate write-in candidates for any of these offices write to the ACA Secretary: Lee Brammer, Department of Chemistry, University of Sheffield, sheffield 53 7HF, UK FAX 44-114 273 8673. Letters must be received by September 15, 2002 and must be signed by five supporting ACA members and include a signed statement by the candidate describing his or her qualifications. Statements from all candidates will be included with the ballots which will be sent to all members in October 2002.

Statement: The Communications Committee has new roles and responsibilities since the change of the ACA Standing Committees in 2001. The rapid growth of information, publications, knowledge and technologies gives us both opportunities and challenges. Better communication will enhance our ability to reach new heights in our research, including communication among ACA members, educating scientists in other fields and the general public, and bringing new developments in technology to the attention of ACA and its members. I am happy to accept this nomination and volunteer my efforts to the ACA. If elected, I am willing to do my best as a member of this Committee.

Contributors to this issue:

Frank Allen, Lonny Berman, Lee Brammer, Jeanette Krause Bauer, Chris Cahill, Charlie Carter, Connie Chidester, Patti Coley, Wally Cordes, Louis Delbaere, Marcia Evans, Phil Fanwick, Marv Hackert, Mary Hammond, Fusen Han, Andy Howard, Kathy Kantardjieff, Lisa Keefe, Patrick Loll, Terry Maquire, Susan Matheson, Steve Muchmore, Patrice Pages, S.N. Rao, Frank Rotella, Melanie Stephenson, Bob Sweet, Iris Torianni, Alex Wlodawer, Winnie Wong-Ng. Special thanks to Christrine Zardecki for the cover and Jeff Deschamps for meeting photos and the collage on page 2.

Andrew J Howard
*Continuing Education
 Committee*



Associate Professor of Biology, Illinois Institute of Technology, 3101 South Dearborn St, Chicago IL 60616 USA

Director, Industrial Macromolecular Crystallography Assoc., Collaborative Access Team, Advanced Photon Source

Education: Ph.D. in physics, UC San Diego, 1981, with Prof. Xuong Nguyen-Huu, B.A. in biophysics, Pomona College, Claremont CA, 1975

Professional activities: member of ACA since 1980, Diffraction Methods in Molecular Biology Gordon Conference: vice-chair 1998; chair 2000, Advanced Photon Source Research Directorate: chair of CAT Directors' Council, 1998-2000

Research interests: Methods development in macromolecular crystallography, particularly data processing software and synchrotron beamline optics, Structural genomics, Pharmaceutical crystallography

Statement: Increasingly, non-crystallographers are using crystallographic tools to pursue their scientific goals. This deprofessionalization of our discipline is a natural correlate of the increasingly central role that three-dimensional structural information plays in modern biology and chemistry, but it comes at a price. Many individuals who need to use sophisticated crystallographic tools (both hardware and software) are unaware of how those tools really operate. My goal as a member of the Continuing Education committee will be to reach out to these non-specialists

to see that the physics and algorithms underlying our techniques are accessible, and to see that the development of crystallographic methods continues in the post-specialist era.

Katherine Kantardjieff
*Continuing Education
 Committee*



W.M. Keck Foundation Center for Molecular Structure (CMoLS), Department of Chemistry and Biochemistry, California State University Fullerton, 800 N. State College Blvd., Fullerton, CA 92834

Education: BS Chemistry/Biology University of Southern California 1979, MS Chemistry/Emphasis Physical Chemistry UCLA 1984, PhD Chemistry/Emphasis Physical Chemistry UCLA 1988

Professional activities: Member, United States National Committee for Crystallography, 2001-2004; Local co-chair ACA Meeting Los Angeles 2001; Member, Executive Committee, Southern California Section American Chemical Society, 1996-2001; Co-Chair, California State University Computational Chemistry Council 2001-2002; Member, Advisory Board California State University Fullerton Bioinformatics Certificate Program; Member, Governing Board California State University Program for Education and Research in Biotechnology.

Research interests: Macromolecular crystallography; small molecule crystallography; structural genomics; bioinformatics; structure-based drug design; crystallographic methods; crystallography education.

Statement: Today's practicing crystallographers are diverse in their background and preparation. In the biotechnology workforce, there is a rapidly increasing need for x-ray crystallographers and individuals skilled in structure-based approaches. Crystallography is a science that encompasses many disciplines, including physics, chemistry and materials science, and at the same time, it provides enabling technology, methodology and information. Still, some members of the research community view crystal structure determination as being too easy and the models so derived as irrelevant beyond the solid state. Therefore, we must continue to teach crystallography, affording both theoretical and practical training in our field. This means not only providing for the professional development of our students and colleagues, but also providing for public education about our field and its significant contributions to modern science.

The W.M. Keck Foundation Center for Molecular Structure (CMoLS) at California State University Fullerton is the first comprehensive x-ray crystallographic and computational facility located in a predominantly undergraduate institution. As CMoLS' Director for nearly 10 years, I have provided faculty, masters' level students and *undergraduates* with opportunities for joint research and education activities directed at the determination and analysis of both small and macromolecular structures. The CSU is the largest public university system in the US, and many students actively participate in research and training by remote access. I have developed successful short courses, tutorials, curricula, instructional texts and public education materials for audiences ranging from university faculty and students to practicing scientists and K-12 teachers. My experience brings to this committee a unique perspective in crystallography education. If elected, I look forward to making valuable contributions to the work of the Continuing Education Committee and to the ACA mission.

Steven W. Muchmore
Data Committee



Group Leader, Computational Structural Biology, Abbott Laboratories Dept. R46Y, Bldg. AP10, 100 Abbott Park Road, Abbott Park, IL 60064

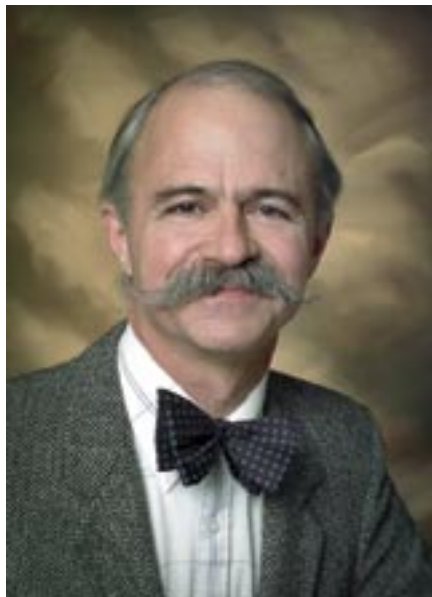
Education: BA (1980), Univ. of Oklahoma, Ph.D. (1996), Purdue Univ.

Research Interests: Use of high-throughput techniques in structural biology and drug discovery, virtual techniques for lead generation, X-ray crystallography and NMR spectroscopy, laboratory automation, structure based drug discovery and design.

Statement: In the last few years, the development of high-throughput techniques have changed the way the information generated by structural biologists is impacting a number of fields. The use of structural information continues to have a significant impact on the rapid generation of compounds as clinical candidates for the treatment of disease. Clearly, the future challenge for scientists in this field will be to maintain a high level of quality while generating the large numbers of data sets that will be possible using the high throughput methodology.

If elected to the Data, Standards, and Computation Committee, I would like to address issues of the standards of quality that should be expected, even when high-throughput methodologies are employed. I view this as an opportunity to ensure that structural biology community will continue to receive a high level of recognition, both in the academic and commercial worlds

Robert M. Sweet
Data Committee



Biophysicist at Brookhaven National Laboratory, Upton, NY 11973.

Education: BS (65) Caltech, PhD (70) Univ. Wisc. Madison.

Professional Activities: Member of U.S. Nat'l Committee for Crystallography. Former chair of Synchrotron Radiation SIG.

Research Interests: Synchrotron radiation, data-collection software and methods, data-harvesting and automated structure

solving, cluster computing, kinetic crystallography, multi-beam diffraction.

Statement: I have spent a significant fraction of my professional career measuring x-ray diffraction data, figuring out better ways to measure diffraction data, or helping others do it. Although data quality is always most important, these days additional issues are becoming significant. As we move to a small-molecule-style, high-throughput paradigm for much of macromolecular crystallography (PX), it is clear we must put effort into the management of data as well as assuring its correctness. For example, in the small-molecule field, the structure-solving process and the result are summarized and recorded more-or-less automatically by the software so that the result can be shipped off for archiving or publication as a CIF file. The PX practitioners are not yet so organized: data must be transcribed from notebooks, log files, scraps of paper, etc. to the final files for PDB or paper writing. In addition to creating new ways to monitor and improve data quality we need to stimulate the use of inexpensive computing clusters. I would use my position on the Data, Standards, and Computing Committee to improve mechanisms to automate harvesting of information during the PX process.

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Crystallography Web Watch

The ACA Communications Committee continues its "Web Watch" in an attempt to keep members informed of useful web sites, primarily of the crystallographic persuasion. While some of these sites may be well known to you, others might not know about them...

Collaborative Computational Projects (CCPs) — The goals of these British-funded projects are to develop, maintain and distribute computer programs and to promote the best computational methods for researchers in biology, chemistry, physics and engineering. Of particular interest to crystallographers are the web sites for CCP4 (protein crystallography): www.ccp4.ac.uk/main.html, CCP13 (fiber and polymer diffraction): www.ccp13.ac.uk/ and CCP14 (powder and small molecule single crystal diffraction): www.ccp14.ac.uk/index.html.

Linux for Crystallography — With the increase in the use of Linux workstations, the number of crystallographic programs that run under the Linux operating system is rapidly expanding. A good place to look for what programs are currently available is in the chemistry section of the WWW Virtual Library: zeus.polsl.gliwice.pl/~nikodem/linux4chemistry.html. Other places with good links to Linux software are the CCP4 newsletter: www.ccp4.ac.uk/newsletter36/11_linux.html and the Stockholm University web site: www.fos.su.se/struc/linux/linuxtal.html.

Crystallographic Software — Network Science has put together a site that lists crystallographic software from A-Z: www.netsci.org/Resources/Software/Struct/xray.html.

ChemSoc — The Royal Society of Chemistry's chemical science network is a wonderfully comprehensive web site. The site contains considerable information, including a lovely visual interpretation of the periodic table and a timeline of events in chemical history, as well as access to conference and society information, IUPAC draft recommendations and career information. Perhaps most useful is a listing of web links to a variety of databases, some of which are explicitly crystallographic: www.chemsoc.org.

Macromolecular crystallization — Looking for a good reference for macromolecular crystallization experiments? Two particularly nice web sites are Terese Bergfors' *Pictorial library of crystallization drop phenomena*: xray.bmc.uu.se/~terese/crystallization/library.html and Johan Zeelen's *X-tal protocols*: www.mpibp-frankfurt.mpg.de/~johan.zeelen//xtal.html.

Have a favorite web site that you'd like to see in a future **Crystallography Web Watch** and possibly linked on the ACA web site? If so, send the web address and a short (1 or 2 sentence) description to Frank Rotella (fjrotella@anl.gov).

Frank Rotella

USNCCr News

The USNCCr met on May 25th, one day before the start of the ACA annual meeting in San Antonio, Texas. New members include Joel Block, James Kaduk, Marilyn Olmstead and Ron Stenkamp. A summary of the recent news concerning the committee and a few important issues that were discussed during the May meeting are described briefly below.

The USNCCr has endorsed William Duax as a candidate for the President of IUCr and suggested Judith Flippen-Anderson as a nominee for the IUCr Executive Committee. The elections will take place at the 19th IUCr Congress in Geneva in August 2002. The USNCCr also recommended names for candidates for various Commission members. These commissions include: Aperiodic crystals; Biological macromolecules; Charge, spin, and momentum; Crystal growth and characterization; Crystallographic teaching; Electron diffraction; High pressure; Neutron scattering; Powder diffraction; Small-angle scattering; Structural chemistry; Synchrotron radiation; and XAFS. The committee has submitted a list of names but is always soliciting additional nominees. It has been suggested that in the future the ACA council and the various SIGs assist in recommending names.

As provided for in the USNCCr By-laws concerning the election of US delegates and alternates to the IUCr Congress in Geneva, a slate consisting of 18 nominees was voted on by the committee members during the USNCCr November meeting in Washington DC. The four elected delegates, who will be led by chair Marvin Hackert, are: Jon Clardy, Bill Stallings, Bob Sweet, and Judy Flippen-Anderson. The five alternates are: Charles Carter, Howard Einspahr, Abe Clearfield, Ian Robinson, and James Kaduk. Plans for the Geneva meeting and the responsibilities of these delegates and alternates was discussed in detail during the May meeting.

The USNCCr has voted to allocate a minimum of \$20,000 in travel funds to support students to attend the Geneva IUCr meeting. The exact amount will depend on the number of applicants. The subcommittee responsible for selecting award recipients is comprised of Kathryn Ely (chair), Ron Stenkamp, Howard Einspahr, one additional member from NASA, and another one from ACA. The detailed logistics of how the funds will be distributed was discussed at the San Antonio meeting.

The USNCCr proposal for funding and support for delegates was submitted by Tamae Wong (Program Director, Board on International Scientific Organizations, NRC) to NSF/MPS. The proposal was packaged with that of several other National Committees. This time we asked for 5-year support, which would be a much more stable arrangement. The NRC leadership is exploring mechanisms that may lead to interim funding while the review process is being conducted. A general discussion about how the USNCCr can best operate was part at the May meeting.

Service Crystallography / Academic Salary Survey 2001

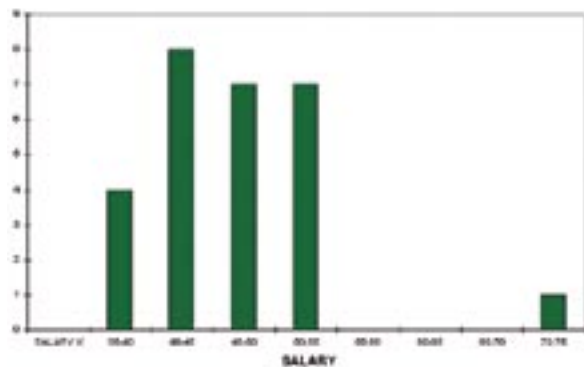
Preparation of the Survey: A survey of salaries and benefits for service crystallographers employed by academic institutions was conducted for the ACA Service Crystallography SIG by Phillip Fanwick of Purdue University. He created the survey which was then edited by past and present officers of the SIG.

Participants: The membership of the SIG was used as the starting point in selecting who could participate in the survey. Those with addresses outside the U.S. and Canada, those with corporate addresses and student and retired members were eliminated from that list. Additional names were obtained from Carol Brock's list of service crystallographers. Finally, past and present officers of the SIG reviewed the list for additions and deletions. The final list consisted of 122 names that included both known service crystallographers and those whose status could not be determined. 122 surveys were mailed out. 34 responses (14 US / 3 Canadian) were received.

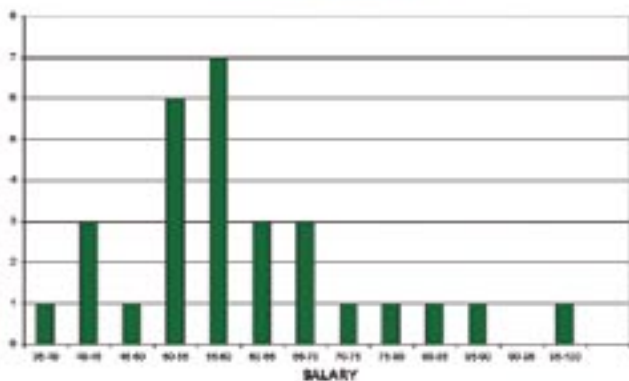
Survey Results:

The charts below displays the results of two salary surveys. In 1996 the mean salary was \$46,463; the median \$45,000; and the standard deviation was \$6,840. In 2001 the mean was \$59,717; the median \$58,000 and the standard deviation was \$13,074.

ACADEMIC SALARIES 1996



ACADEMIC SALARIES 2001



Comments on salary ranges: First, as reflected in the increase standard deviation the results in 2001 cover a wider range than in 1996. The increase in the mean represents a 5% compounded yearly increase. In 1996, the Canadian average salary was \$45,444 in Canadian dollars. Because only three surveys were received in 2001 it was not possible to determine a reliable average. The average of those received was \$42,374.

What crystallographic services do you typically perform:

- a. crystal Growth 13%
- b. crystal mounting 100%
- c. data Collection 100%
- d. structure solution and refinement 97%
- e. graphics 97%
- f. publication preparation 90%
- g. instrument maintenance 100%
- h. programming 61%
- i. teaching crystallography 74%
- j. Other : included working with computers (web development, system manager, etc.) 23%; teaching courses outside of crystallography 10%; and other 6%

Travel :

In the past university support for travel has paid:

- a. all expenses 60%
- b. almost all expenses 10%
- c. a majority of expenses 17%
- d. a few expenses 10%
- e. nothing 3%

University support for travel has allowed you to:

- a. attend any scientific meeting or other event 10%
- b. attend 2 or more meetings a year 32%
- c. attend 1 meeting a year 42%
- d. not attend meetings 10%
- e. never tried to obtain university funding 6%

With regards to the upcoming IUCr meeting:

- a. universty will cover all expenses 13%
- b. universty will cover majority of expenses 6%
- c. majority of support from other sources 6%
- d. will not attend because of insufficient support 26%
- e. no intention of attending regardless of support 39%
- f. university never funds international travel 10%

Travel Support (multiple answers allowed):

- a. yearly budget under your control 39%
- b. provided as needed 48%
- c. external grants 16%
- d. internal grants 0%
- e. Other 6%

Facilities:

Office space provided to you is:

- a. in a room not separate from the x-ray facilities 71%
- b. enclosed office totally within the x-ray facility 23%
- c. an open space in the x-ray facility 6%
- d. no office space is provided 0%

Comment: Due to a proof reading error the first answer should not contain the not. Some answered a with the not crossed out while others simply selected a.

With regard to the size of the x-ray facility:

- a. sufficient space for now and for future growth 35%
- b. sufficient space for now but no room for growth 48%
- c. current space is marginal for current needs 10%
- d. current space is inadequate for current needs 6%

With regard to the appearance and condition of the x-ray facility as compared to other research facilities within your department/institution:

- a. outstanding — a real show place 23%
- b. as good as other similar labs and facilities 61%
- c. ok but not as good as other labs and facilities 10%
- d. a disgrace 6%

Is the x-ray facility shared with other research facilities?

Yes 23% No 77%

Charges and Services

The average cost for a typical structure by an on-campus user is: mean \$234, median \$200, standard deviation \$218. Low was \$0 and high was \$1,000.

Do you charge non-academic users unaffiliated with your institution more?

Yes 90% No 0% NA 10%

Do you provide Powder Diffraction Services?

Yes 32% No 68%

Philip Fanwick

ACA folks caught hard at work in San Antonio



ACA Data, Standards & Computing Committee: Victor Young, John Huffman, Jeff Deschamps and Helen Berman



ACA Service SIG: Michael Carducci (Secretary) and Richard Staples (Chair-elect)



ACA Small Molecule SIG: Brian Patrick (Chair-elect), John Bollinger (Chair) and Joe Reibenspiet (Secretary)



Simon Billinge (Chair - Neutron Scattering SIG), Paul Butler (Chair, Small Angle Scattering SIG) and Scott Misture (Chair, Materials Science SIG)

Cover Story - The Art of Science - Images from the Protein Data Bank

The recent exhibit “The Art of Science – Images from the Protein Data Bank,” highlighted various representations of macromolecular structures to show the beauty inherent in their three-dimensional structure. Held at The Gallery, a space dedicated to art exhibits at Rutgers, The State University of New Jersey, a mix of undergraduate and graduate students, professors, and local educators made the exhibit one of the Gallery’s most popular productions.



Opening reception for “The Art of Science” exhibit at Rutgers University.

large-scale depictions of the molecules were taken directly from the entry’s Structure Explorer page (www.pdb.org/). Images of collagen by Jordi Bella, assistant research scientist at the University of Manchester, and illustrations from the PDB’s Molecule of the Month series by David Goodsell, assistant professor of molecular biology at the Scripps Research Institute, were also in the show.



PDB Annotator Tania Rose Posa and the wall of proteins.

As noted by the New Jersey’s *The Star-Ledger* and *The Bergen Record*, many guests to the exhibit were surprised by how they were attracted to the beauty of the images, which in turn inspired their interest in the scientific descriptions that accompanied the pictures.



Kyle Burkhardt (PDB Senior Annotator) and virus structures (Molecule of the Month: August 2001).

The goal of the exhibit was to introduce these beautiful shapes of macromolecules to the Rutgers community. For the Gallery’s generalized audience, the images were selected for their strong visual component. Magnified and mounted, the colorful presentation drew attention to the fascinating shapes of the structures, such as the long strands of collagen and the spherical shells of viruses. Accompanying captions referenced the structure and provided some introductory information. The



Rutgers Associate Dean Edmund Scheer and Molecules of the Month: actin (July 2001) and myosin (June 2001).

The PDB would like to see this exhibit travel to other places. If you would be interested in sponsoring this exhibit at your institution, please contact the show’s curator Christine Zardecki at zardecki@rcsb.rutgers.edu. The PDB is supported by funds from the National Science Foundation, the Department of Energy, and two units of the National Institutes of Health: the National Institute of General Medical Sciences and the National Library of Medicine.

Christine Zardecki

The Brazilian National Laboratory for Synchrotron Light

The first synchrotron light source to be constructed in the Southern Hemisphere was officially opened to users on 1 July 1997. The source is based on a 1.3 GeV electron storage ring designed and built by laboratory staff. LNLS has 10 beam lines that collectively span the photon spectrum from 10 eV to more than 10 keV. Beam lines are available for x-ray structural and spectroscopic studies--including small-angle scattering, diffraction, fluorescence, absorption spectroscopy, protein crystallography, and deep lithography--as well as for ultraviolet and soft x-ray spectroscopy. New beam lines for x-ray powder diffraction and infrared spectroscopy are in the planning stages. The beam lines, like the storage ring, were designed and built in-house. More than 500 projects have been performed at LNLS since its opening. Although 80% of the projects originated within the Brazilian scientific community, a significant fraction (15%) were led by scientists from neighboring Argentina, who have free access to the facility. Other projects have come from several countries in the Americas and Europe, and strong emphasis is given to international collaborations within Latin America. Materials scientists are the largest segment of users, followed by biologists, physicists, and chemists.

The facility was built by the Brazilian Council for Scientific and Technological Development, and is now funded by the Ministry of Science and Technology. Management is by the Brazilian Association for Synchrotron Light Technology, a private, nonprofit organization which also manages two other facilities on the LNLS campus: a National Center for High Resolution Electron Microscopy, the centerpiece of which is a 300-keV transmission electron microscope, and a new Structural Molecular Biology Center.

With more than 150 staff members, superb technical infrastructure, and more than 14000 square meters of laboratories and auxiliary facilities, LNLS is a world-class facility and is the largest and most modern national laboratory for materials and biological research in Latin America.

Excerpted from "Physics in Latin America Comes of Age", by Jose Luis Moran-Lopez, Physics Today 53 (10) Copyright 2000. American Institute of Physics

Opportunities for Learning at LNLS

The LNLS organizes courses, workshops, training programs and summer schools. Every year there is a Users Meeting, where the results of the projects that have been performed during the year are presented. A number of graduate students perform their thesis work in the different experimental facilities of the synchrotron light source. Post-doctoral fellows, endowed by the State and National Research Foundations find excellent opportunities to develop their research programs at the LNLS.

Iris L. Torriani

Financial Aid for Latin American Researchers at the LNLS

This program was started in 1999 and will finance the air ticket (**roundtrip**), from the country of origin to the city of São Paulo or Campinas **for the main researcher** whose project has been approved by the Scientific Committees of the LNLS, in areas of research related to applications of synchrotron light. **The total aid** includes, in addition to travel expenses, lodging for the researcher in the Guest House of the LNLS and lunches during the period assigned for execution of the project. Specific rules for this program are found at the site of the LNLS: www.lnls.br.

Iris L. Torriani

Crystallography at the Spring AGU Meeting, Washington, DC, May, 2002

The MSA Mineral Structures SIG hosted a workshop entitled "Freely available crystallographic software for mineralogists" during the American Geophysical Union's Spring Meeting in Washington, DC (May 28th - 31st, 2002). The group, which included attendees from academia, industry, government offices and museums, gathered at the Smithsonian Institution's National Museum of Natural History to hear some informative presentations by Lachlan Cranswick. Lachlan is the Secretary of the Collaborative Computational Project Number 14 (or CCP14) and maintains a website of freely available programs for crystallography. Aside from telling how to get these programs, Lachlan also evaluates the software and writes highly valuable tutorials on their use. A very detailed 'how-to' on using Brian Toby's GSAS GUI was also presented at the workshop and certainly brought many of us up to date. Notes from this presentation can be found at the CCP14 website: www.ccp14.ac.uk/index.html. The workshop concluded with a reception in the famous 'Blue Room' of the National Gem and Mineral Collection. Cool drinks were enjoyed during a show-and-tell of recent specimen acquisitions and some of the not-so-open-to-the-public holdings. Jeff Post and his colleagues are to be commended on their hospitality.

There was also a Mineral Structures and Stabilities poster session at AGU; Jeff Post and Peter Burns, presiding. While more sparsely attended than in recent years, the session nonetheless had thirteen exciting posters on a number of new structures. Highlights included some clever use of a CCD based diffractometer by Andrew Locock (Notre Dame) to collect data on autinite, a uranyl phase prone to rapid dehydration, and recent results from soft-mode phase transition studies in orthoenstatite by Jennifer Jackson (U. Illinois, Urbana-Champaign).

Chris Cahill

RapiData 2002, Brookhaven National Laboratory, April 21-26

Brookhaven National Lab's offering of RapiData 2002, the fourth in an annual series of crash courses in crystallography, was once again a huge success. Forty-eight students from around the world participated from April 21 to 26. More formally titled "Rapid Data Collection and Structure Solving at the NSLS: A Practical Course in Macromolecular X-Ray Diffraction Measurement," the program was developed by BNL's Biology and National Synchrotron Light Source (NSLS) departments to introduce students to the best people, newest equipment, and latest techniques in the field of macromolecular x-ray crystallography.

Half the students came to observe; the other half came with their own specimens with the goal of solving the structure of a particular enzyme. About four structures were solved during the course, and each of these is likely a publishable result.

The program was designed and run by Bob Sweet and Denise Kranz of BNL's Biology Department. The course starts with two days of lectures and tutorials, taught by BNL scientists and volunteer scientists from industry. The lectures focus on the connected themes of data collection and structure solving. There are five lectures on fundamentals of data collection and instrumentation. Two specialists lecture on preparation of cryocooled crystals. There are three different data-reduction packages presented. Finally there are four lectures on the fundamentals of different software packages for the solving of structures.

After the lectures, the students move to the NSLS beam lines to begin collecting data on their crystal samples for the next two and a half days. There were 38(!) instructors, tutors, or helpers: thirteen from BNL Biology, three from the NSLS, eight from various industrial groups (roughly half of these are equipment sales persons, half just volunteers who come for the fun of it), and 14 others from academia and other national labs. Nearly all of the lectures on software were amplified in tutorials and on-line demonstrations during the data collection, and there also are plenty of occasions for conversation over drinks and meals.

Everyone, teachers and students alike, find the experience absolutely riveting. The 60 hours of data collection are near chaos on the NSLS floor. Each of us ends up exhausted but happy, having learned a little from each of the others.

This year, to amplify its Latin American Initiative, the U.S. National Committee for Crystallography provided some funds for partial travel scholarships to the course for six students, three from Brazil, two from Mexico, and one from Argentina.



Latin American Students: (back from left) Enrique Rudino-Pinera (Mexico), Ariel Edgardo Mechaly (Argentina), Hannes Fischer (Brazil), Frederico Moraes Ferriera (Brazil); (front from left) Rogerio Sotelo-Mundo (Mexico), Adriana Lucely Rojas Cardona (Brazil); and Robert Sweet, BNL Scientist.

The course is funded by a range of agencies, with the key support coming from the National Institutes of Health National Center for Research Resources, and significant support from the U.S. Department of Energy's Office of Biological and Environmental Research. For more information about this year's program, including the sources of funding, go to: www.px.nsls.bnl.gov/

Bob Sweet

ICDD Annual Spring Meetings



ICDD officers and directors: (front row) Evgeny Antipov, Terry Maguire, Julian Messick, Cam Hubbard, Tim Fawcett, Brian O'Connor, David Rendle. (back row) Bob Snyder, Jim Kaduk, Ray Goehner, Daniel Louer. (missing) Ron Jenkins

During the week of 18-22 March 2002, the International Centre for Diffraction Data (ICDD) welcomed its members to the headquarters office in Newtown Square, Pennsylvania for its Annual Spring Meetings. An international gathering of the ICDD members, representing a wide range of scientific disciplines, participated in the various committee, subcommittee, and task group meetings held throughout the week. The members play an essential role in the development of the ICDD, its database products, and services, tailoring those products and services to the needs of the global scientific community. In addition, the ICDD Board of Directors met to discuss the financial, business, and long-range planning functions of the ICDD.

The following meetings were held:

Task Groups: Ceramic Task Group, Financial Support Task Group, Metals & Alloys Task Group, Merck Task Group, X-ray Diffraction Task Group.

Subcommittees: Ceramics, Education, Electron Diffraction, High Pressure/Temp. Diffraction, Marketing, Metals & Alloys, Minerals, Organic & Pharmaceutical, P.D.F. Editorial Staff, Polymers, X-ray Diffraction Methods.

Committees: Awards, Bylaws, Employee Benefits, Finance, Grant-in Aid, Long Range Planning, Ludo Frevel Scholarship, Membership, Technical.

On Wednesday evening, 20 March 2002, a technical poster session was held, presenting a forum for members to discuss various interest areas and recent developments in X-ray diffraction. The ICDD sponsored a mixer along with the poster session.

The Technical Committee meeting on Thursday, 21 March 2002, served as a forum for summarizing all subcommittee activities and included reports by ICDD's Regional Co-chairs: Shao-Fan Lin (China); Nubuo Ishizawa (East Pacific Rim); David Taylor (England); David Rafaja (European Community); James A. Kaduk (North America); Evgeny Antipov (Russia); José M. Delgado (South America); and Brian H. O'Connor (Southeast Asia). The co-chairs reported on activities related to

the ICDD and on activities in the region that would be of general interest to the X-ray analysis community. Results of global X-ray conferences, workshops and clinics were described as well as proposals for future activities in each region. In a typical year, the ICDD financially supports or directly conducts over a dozen forums for X-ray analysis technology exchange across the globe.



Terry Kahmer, Vesna Bosnic, and Charlie Prewitt at the poster session

The Annual Meeting of Members was also held on Thursday, where Cam Hubbard, ICDD's Chairman, discussed the high productivity and major progress on the Powder Diffraction File®, and the overall evolution of ICDD over the last several years. This year, the ICDD will release two new commercial products, designed to bring unprecedented database capabilities to the global X-ray diffraction scientific community. The first product, to be released in May, contains 136,800 materials and is the next generation of the historic Powder Diffraction File (PDF®) – PDF 4/Full File 2002. The second product, a collaborative effort with the Cambridge Crystallographic Database, is to be released in November and contains 146,000 organic and organometallic materials – PDF 4/Organics 2002. Both databases are in a relational database format that allows complex Boolean search

queries of more than 30 separate fields. This format allows users to search on diffraction data (d's, I's), unit cell parameters, chemistry, melting points as well as a wide range of physical and optical properties and bibliographic references. Combined, these databases contain 257,000 unique entries, which can also be searched by material subsets such as pharmaceuticals, minerals, metals & alloys, polymers, superconductors, zeolites, etc.



Tom Blanton, Chair of the Grant-in-Aid Committee, presented Distinguished Grantee award to Evgeny Antipov.

Evgeny Antipov, Moscow State University, received the Distinguished Grantee Award and also gave a presentation of his work in the ICDD Grant-in-Aid Program, which includes reference patterns for industrially important, advanced inorganic materials. Dr. Antipov was also cited for the high quality of his contributions to the PDF and his role in the development of the powder diffraction community in his region. The retiring members of the Board, Jeffrey N. Dann, Charles T. Prewitt, and Jeffrey E. Post were recognized for their service. As per the results of the recent election of officers and directors, the new slate of directors serving the term 2002 –2004 was also announced:

Chairman: *Camden R. Hubbard*
Vice Chairman: *Brian H. O'Connor*
Treasurer: *Julian Messick*
Corporate Secretary: *Terry Maguire*
Executive Director: *Timothy G. Fawcett*
Chairman, Technical Committee: *James A. Kaduk*
Directors-at-Large: *Evgeny Antipov, Raymond P. Goehner, Ron Jenkins, Daniel Louer, and David F. Rendle*
Past Chairman: *Robert L. Snyder*

Interested in becoming an ICDD member? Please visit our web site at www.icdd.com, or contact our Membership Committee Chairperson, Dr. Winnie Wong-Ng, at wongng@icdd.com.

Terry Maguire

Brookhaven Draws Record Attendance for Annual NSLS Users' Meeting

This year's Annual National Synchrotron Light Source (NSLS) Users' Meeting, held at Brookhaven National Laboratory (BNL) on May 20-22, was characterized by exciting presentations about the successful scientific record of the past year, plans for upgrades of the NSLS and a new light source facility, and a record attendance of 380 participants coming from all over the world. The meeting consisted of a one-day plenary session and eight one-day-long workshops on the latest results achieved at the NSLS in the physical, biomedical, environmental, and instrumentation sciences. Leemor Joshua-Tor of Cold Spring Harbor Laboratory served as Chair of the entire event. Lonny Berman of NSLS served as the Program Chair for the plenary session, and Anatoly Frenkel of Yeshiva University served as the Workshops Chair.



Attendees of the Workshop on Practical Aspects of Membrane Protein Crystallography: From Overexpression to Crystallization. Kneeling in front are session organizers Fillippo Mancina (center) and Larry Shapiro (right).

During the plenary session, NSLS Chairman Steven Dierker presented recent upgrades and future projects at the NSLS, and Richard Osgood, Associate Laboratory Director for Basic Energy Sciences, showed how the future Center for Functional Nanomaterials at Brookhaven would serve the NSLS user community as well as other potential users.

John Marburger, President George W. Bush's Science Advisor and Director of the Office of Science and Technology Policy (OSTP), was the meeting's keynote speaker. He described how current and future scientific capabilities will shape science and technology in the 21st century, and how the NSLS will play a role in this endeavor.

During the workshops and part of the plenary session, scientists presented their current research as well as future light source projects. The workshops addressed topics as diverse as the use of synchrotrons in the environmental sciences, the study of ultrafast processes with x-rays, nanoscale materials, membrane protein crystallography, catalysis, materials processing, synchrotron micro-spectroscopy and imaging, and the development of more advanced light source detectors.

The future of the NSLS and the proposed Nanocenter at Brookhaven

In his keynote address, Marburger said, "We are beginning the 21st century with a profound revolution in science based on capabilities in computing and instrumentation. These capabilities have achieved an importance as the foundations of contemporary

science that earns them a top priority for support. The National Synchrotron Light Source is one of the key representatives of this new instrumentation."

Steven Dierker highlighted the qualities that make the NSLS such a successful facility. "With more than 2,500 scientists from over 400 institutions per year coming from academic, industrial, and government institutions, the NSLS is a widely used facility," he said. "Not only do we have a large contingent of users, but, last year, they also produced more than 800 publications based on research performed at the NSLS, 150 of which appeared in premier science journals."

In terms of budget, Dierker announced that the Department of Energy (DOE) had recently added \$600,000 to the NSLS budget for FY02. An additional \$1.6 million is also contained in the President's FY03 budget request. "Altogether, we are looking at an increase of \$2.2 million next year," Dierker said. "We are very grateful to DOE and Congress, and we are excited about the opportunities that this additional funding will allow."

Dierker also discussed changes under way at the NSLS that will improve support for current and future users. One major change has been an administrative reorganization, to provide better coordination for project management and to place greater emphasis on support for user science. "We expect these changes to increase productivity and to enable our users to obtain better research results," Dierker said.

Future plans also include upgrades of beamlines on the VUV

and X-ray storage rings, such as an increase of insertion devices, the redesign of radio-frequency cavities and end stations, and development of new beamline scientific programs.

“We really would like to free up our users to spend more of their time, energy and resources focusing on doing their science,” Dierker said. “We expect these changes to increase productivity and to enable our users to obtain better research results.”

In announcing longer-term plans, Dierker first hailed a recent achievement by one of the near-term future light sources, the deep ultraviolet free electron laser (DUV-FEL). Last February, the facility generated radiation at 400 nanometers (billionths of a meter) by a process called self-amplified spontaneous emission process. By fall, Dierker added, the DUV-FEL is expected to provide radiation at 88 nanometers, to be used in pioneering chemistry experiments.

To improve the current performances of the NSLS by increasing beam brightness while reducing its pulse length, Dierker announced two approaches for a new facility. The first approach is based on an ultra-low emittance storage ring, and would provide about a factor of 10,000-increase in brightness. The second approach, the Photoinjected Energy Recovery Linac (PERL), would produce high brightness (on the order of 10^{21} ph/sec-mm²-mrad²-0.1% bandwidth), about a factor of 100 better for coherence, and very short (sub-picosecond) pulse lengths.

Because of technical challenges facing the construction of PERL, Dierker suggested that an intermediate approach between a storage ring and PERL would be the most reasonable design for a future light source at BNL. “The design would start with an ultra-low emittance storage ring, and evolve toward a PERL approach as that technology develops,” he said. “This new ring, which would take at least two years to build, would be located adjacent to the x-ray ring.”

During her presentation on the current programs managed by the DOE Office of Basic Energy Sciences (BES), Patricia Dehmer, Associate Director of Science for BES at DOE, was enthusiastic about the current and future projects at the NSLS. “I am delighted by the way Steve Dierker has done a tremendous job over the past year in rethinking the challenges that face the NSLS,” she said.

U.S. Representative Felix Grucci (R-NY), who was scheduled to speak at the meeting, was detained in Washington. In a message read by Meeting Chair Leemor Joshua-Tor, he praised the current and future scientific programs at the NSLS.

Another new project discussed at the meeting was a center dedicated to the study of the infinitesimally small. Called the Center for Functional Nanomaterials, or Nanocenter, for short, this new BNL facility, which will investigate materials a billionth of a meter in size, has received a “very strong thumbs up” from initial reviews by DOE-BES, according to Satoshi Ozaki, Special Assistant to the BNL Director for Accelerator Projects, who gave the meeting’s welcoming address.

“The Nanocenter will be organized in a way that is very similar to the NSLS,” said Richard Osgood. “The center will include laboratory clusters, user and visitor laboratories, and training

and seminar facilities. Each of the lab clusters will work like a beamline, with scientists performing various functions, such as growing materials, patterning materials, and looking at them with electron microscopes.”

Now in its latest stages of approval by DOE, the Nanocenter is expected to be built close to the NSLS and the BNL Instrumentation Division. “The NSLS and the Nanocenter will be portals to each other,” says Osgood, who masterminded the Nanocenter project since its inception. “We envision both of these facilities as helping each other in maintaining a strong and vigorous user base.”

“Brookhaven’s Nanocenter will be a very bold departure from business as usual in the research communities of materials sciences and chemistry,” Dehmer said. “We are trying to change the face of small science by co-locating a lot of disciplines in one place, so that if scientists want to pursue a research program that mixes chemistry, biology and materials science, they can do it all in one place.”

In his keynote address, Marburger described the new changes facing science in the 21st century. “Scientists are opening the doors to a new kind of science,” he said. “Never before had we been able to relate properties of large-scale matter and big things made of atoms to their detailed atomic structure. Now, we can, and the prospects are truly exhilarating. A wide landscape of opportunity has opened before us, promising unprecedented richness of discovery.

“I look forward to seeing what comes out of this laboratory as well as the others that I fully expect society to continue to support,” Marburger concluded.

The increasing emphasis of life sciences as an important NSLS program component was reflected in the afternoon portion of Tuesday’s plenary session, which was divided into sessions focusing on structural biology and biomedical research, each of which opened with a presentation by a representative of the National Institutes of Health (NIH). The structural biology session led off with a presentation by Judith Vaitukaitis, the Director of the National Center for Research Resources (NCRR), which funds two biomedical research resources at the NSLS. The biomedical research session led off with a presentation by Richard Swaja, the Acting Director of the Division of Biomedical Imaging of the newly-created National Institute of Biomedical Imaging and Bioengineering.

Latest results from light source research and future applications

During the plenary session on Tuesday, light source scientists presented some of the latest results in condensed matter, structural biology and biomedical research, as well as future x-ray applications.

NSLS scientist Ron Pindak showed how resonant x-ray scattering could be a unique probe of the changing orientational order that underlies the morphology of phases exhibited by rod-shaped and banana-shaped liquid crystal molecules.

Neurobiologist Roderick MacKinnon, of Rockefeller University in New York, presented the structure (using x-ray crystallography)



At right: Science Advisor John Marburger. Next to him in front: Leemor Joshua-Tor (incoming Chair of the NSLS Users Executive Committee). Holding the sign and behind them are from left to right: Satoshi Ozaki, Richard Osgood, Steven Dierker, Patricia Dehmer, and Simon Bare (outgoing Chair of the NSLS Users Executive Committee).

and function of ion channels and associated regulatory proteins. His research is directed at understanding the molecular mechanisms of ion channels, which are involved in the pace of the heart, hormonal secretion, and the electrical impulses of neurons. The ultimate goal of his research effort is to solve the complete structure of the ion channels under study.

Environmental questions addressed with synchrotron light

A workshop on applications of synchrotron radiation in the environmental sciences has become a tradition at the meeting. This year's was organized by Douglas Hunter of the Savannah River Tech Center. Two talks were given on powder diffraction. Jeffery Post, Curator of the National Gem and Mineral Collection of the Smithsonian, demonstrated his joy in basic research by discussing real-time powder diffraction studies of the dehydration behaviors of clays. Geoscientist Peter Heaney, of Pennsylvania State University, showed how real time powder diffraction studies of hydrotalcites could elucidate the mechanism of rapid cation exchange in this class of clay minerals.

New insights into cell membrane proteins

Integral membrane proteins perform some of the most important functions of living cells, yet understanding their molecular mechanisms through structural studies presents unique challenges. A workshop whose aim was to discuss the nuts-and-bolts of over-expressing, purifying, and crystallizing membrane proteins for structural studies by x-ray crystallography was organized by Larry Shapiro and Filippo Mancina of Columbia University. This was the most popular of the 8 workshops.

Biologist Susan Buchanan, of the National Institute of Diabetes and Digestive and Kidney Diseases (NIDDK) at the NIH in Bethesda, made a presentation on the production, purification, and characterization of bacterial outer membrane proteins both refolded from inclusion bodies and also as membrane-inserted functional proteins.

Cell biologist Da Neng Wang, of New York University, described the production

of bacterial inner membrane transporters as functional affinity-tagged proteins, and methods for optimization of each step in their production and purification.

Biologist Martine Cadene, of Rockefeller University, explained the use of the Matrix Assisted Laser Desorption Ionization (MALDI) mass spectrometry in defining the covalent state of purified membrane proteins, and use of this information as an aid in designing mutant constructs specifically amenable to crystallographic analysis.

Biologist Miro Venturi, of NIH, described methods for the production and screening of monoclonal antibodies specifically reactive against the folded conformations of integral membrane proteins. He described recombinant methods for production and purification of Fab and Fv fragments of these antibodies, and their use as crystallization reagents, giving work with the transporter protein NhaA as a specific example.

Structural biologist Reinhard Grishammer, of NIH, gave a detailed presentation on the expression and purification of functional G-protein coupled receptors as fusion proteins in *E. coli*. He gave examples of success with this approach for several different GPCRs.

Barry Springer, director of Molecular Biology and Protein Biochemistry and project team leader at 3-Dimensional Pharmaceuticals Inc. (3DP), presented the expression of functional GPCRs in mammalian (HEK-293) cells, and biophysical and fluorimetric high-throughput assays to assess their functionality and stability in detergent-containing solutions.

Biophysicist Ehud Landau, University of Texas Medical Branch in Galveston, described the use of cubic lipidic matrices as a medium for the stable incorporation of integral membrane proteins, and their crystallization in this medium. He presented many examples of highly diffracting crystals obtained using this methodology.

BNL biologist Dax Fu described the stabilization of solubilized bacterial transporters by inclusion of their cognate binding ligands, a necessary precursor to their successful crystallization.

Biochemist Patrick Loll, of Drexel

University, presented a rational approach to the design of crystallization screens for membrane proteins, based on the “cloud points” of detergents in different protein-precipitating conditions. Based on this approach, he has developed screens containing over 600 potentially useful conditions, near detergent phase transitions, and demonstrated a high rate of success with this screen.

Catalysts' secrets revealed

In a successful and informative workshop titled “Recent Advances in the Application of Synchrotron Radiation to Catalysis”, organized by Simon Bare of UOP, topics ranged from new developments of using soft x-rays at high pressures to in situ x-ray diffraction (XRD) studies.

BNL chemist Jon Hanson highlighted the applicability of in situ XRD for following structural phase transformation in bulk catalysis.

Light Source imaging techniques galore

One of the most well attended workshops at the meeting focused on imaging and micro-spectroscopy. The goal of the workshop was to introduce and describe the many micro-spectroscopy and imaging techniques available at the NSLS, including infrared (IR) micro-spectroscopy, hard x-ray microprobe, scanning transmission x-ray microscopy (STXM), x-ray micro-diffraction, diffraction-enhanced imaging (DEI), and x-ray micro-tomography. The workshop provided unique insight into why the NSLS is so well suited for these techniques. It was organized by Lisa Miller of NSLS and Antonio Lanzirrotti of the University of Chicago.

The synchrotron light produced at the NSLS is 1,000 to 10,000 times more intense than that produced at conventional laboratory sources. The light is also very highly collimated and covers a broad spectra range, from x-ray wavelengths as small as 0.1 Å to the far-infrared, with wavelengths longer than 107 Å.

These characteristics mean that smaller, more intense beams can be produced, giving scientists the capability to produce images of extremely small or dilute samples, determine elemental or molecular concentration gradients, and probe the chemical states of elements and compounds in a variety of materials with very high spatial resolution.

The workshop gave attendees a practical sense of the individual techniques available to them and specific examples of how such techniques are being used and combined by users to solve complex scientific problems in a variety of fields.

Physical chemist Jean Jordan-Sweet, from the IBM Research Division's Thomas J. Watson Research Center in Yorktown Heights, introduced the attendees to the uses of micro-diffraction imaging at the X20 beamlines, showing how these instruments can be used to study interfacial strain caused by residual stresses in materials and for real-time characterization of electro-migration effects with a spatial resolution as small as 2 μm.

NSLS physicist Zhong Zhong highlighted the recent and dramatic advances in diffraction-enhanced imaging (DEI) at the X15A beamline. DEI dramatically enhances the ability to

image and contrast soft tissue in ways not currently possible using techniques such as magnetic resonance imaging (MRI) and computed tomography (CT) imaging. In the field of clinical imaging, particularly with respect to mammography, it's clear that DEI can provide remarkable sensitivity compared to standard radiographic techniques.

Geophysicist Russell Hemley, of the Carnegie Institute in Washington, DC, presented studies of high-pressure materials and compounds using FTIR and x-ray micro-diffraction techniques.

Watching materials as they grow and change

A workshop titled “In situ studies of materials processing”, organized by Karl Ludwig of Boston University, Randy Headrick of the University of Vermont, and Chi-chang Kao of NSLS, included speakers who use synchrotron-based x-ray techniques to study materials processes and speakers from outside the synchrotron community.

Physicist Randy Headrick kicked off the workshop with an overview of in situ studies of materials processing. He outlined the information that can be obtained with different synchrotron-based surface x-ray techniques and assessed the potential of NSLS wiggler beamline X21 for such studies in the future.

Physicist Christian Lavoie, from the IBM Research Division's Thomas J. Watson Research Center, showed how the use of real-time synchrotron light can dramatically reduce the time necessary to investigate the physical properties and transformations in a wide range of cobalt alloy silicides.

Materials scientist Kit Umbach, of Cornell University, showed how grazing-incidence small-angle x-ray scattering (GISAXS) had enabled him to follow carefully the formation of ripple patterns on silicon dioxide during sputter erosion with argon ion beams. His results suggest that the finite viscosity of the surface plays an important role in determining the surface morphology.

This work contrasted with that of materials scientist George Malliaras, of Cornell University, who is developing pentacene-based optoelectronic materials. His initial atomic force microscopy (AFM) and x-ray scattering results with Headrick suggest that there is an unusual structure in the first layer of pentacene deposited onto silicon, and that 3-d crystallites nucleate on top of that layer. One of the most powerful surface x-ray techniques is surface crystallography, but its effective utilization requires solving the well-known phase problem.

Physicist Paul Lyman, of the University of Wisconsin in Milwaukee, showed that, to some extent, this problem could be overcome by using maximum entropy methods.

The last three talks dealt with very important materials processes for which real-time x-ray scattering may be able to provide vital information.

Physicist R.D. Vispute, of the University of Maryland, discussed the extensive pulsed-laser deposition (PLD) growth efforts at his university, focusing particularly on efforts to develop aluminum nitride dielectric layers for use on silicon-carbide-based devices

30th Mid-Atlantic Protein Crystallography Workshop, May 2-4, 2002

The 30th Mid-Atlantic Protein Crystallography Workshop took place on the Frederick campus of the National Cancer Institute on May 2nd-4th, 2002. This annual meeting brought together over 120 participants from various crystallography laboratories from North Carolina, Virginia, Maryland, and New Jersey. The exciting opening lecture on “Domain swapping, amyloids, and proteins” was given by David Eisenberg (UCLA). Nineteen other contributed talks and 15 posters covered such varied areas as the structures of known and hypothetical enzymes, DNA-binding proteins, and immune system proteins, as well as technical aspects of crystallography such as molecular replacement, data acquisition and analysis, and “Fun and easy graphics to analyze and fix your structure”. The closing lecture by Mariusz Jaskolski (A. Mickiewicz University, Poznan, Poland) covered the exciting atomic-resolution structures of two trypsin inhibitors.



Gershon Cohen (NIH), Cathy Klein (Rigaku/MSU) and Fred Dyda (NIH)

Exhibitors from Rigaku/MSU and Bruker AXS showed their latest wares and provided much needed liquid refreshments for the participants.



Marcin Paduch, Agnieszka Mateja, Arek Olesky, Mary Lewis and Tomek Ciericki (all from UVA) enjoy a picnic lunch during the meeting.

The next meeting in this long-running series will take place next spring at Duke University. It will be organized by David and Jane Richardson and Lorena Beese.

Alexander Wlodawer / Susan Matheson

Bede Laboratory opens at the University of Cambridge in Collaborative Venture

On 7 January 2002, the new Bede Laboratory at the Department of Earth Sciences, University of Cambridge, UK, was opened by Dr Keith Bowen FREng FRS, Group Director of Technology of Bede plc, as a collaborative venture with Professor Ekhard Salje FRS and his team of scientists at the University.

The University is providing a dedicated laboratory to accommodate three Bede instruments, located within the Dept. of Earth Science’s existing X-ray Diffraction Suite. Bede plc is loaning an advanced research D1 diffractometer incorporating a Microsource® generator and Bede’s analytical software, together with providing support for a research technician and a contribution towards the running expenses for the Laboratory.

The relationship between Bede and the Department of Earth Sciences began two years ago when Bede delivered a Bede Microsource® X-ray generator to Professor Salje for evaluation. Professor Salje and Dr Simon Redfern were so impressed with the revolutionary design of the small, compact system which offers high intensity at low power, that they ordered three for use by the University.



Dr. Keith Bowen and Professor Ekhard Salje cut the ribbon to open the new laboratory

X-ray generators are also incorporated into the other two instruments in the Bede Laboratory at Cambridge, namely a high pressure powder diffractometer with an INEL detector and a combined XRD-thermal analysis instrument, both designed by Professor Salje and his team. The three instruments will be able to establish the capabilities of the Microsource® in novel and demanding powder diffraction applications.

Professor Ekhard Salje said: “The Department of Earth Sciences has a worldwide reputation for work in the field of advanced diffraction technology with several novel types of instrumentation developed by the department. Forging a partnership between these two institutions is an exciting new venture with great potential for innovation and novel applications of X-ray diffraction.”

Dr Keith Bowen said: “We are delighted to form a partnership with this world class team which is applying X-ray diffraction to problems in geology, mineralogy and the chemical and pharmaceutical industries.”

Melanie Stephenson

Travel Grant Awards for ACA San Antonio

North America

Chris Banchs -Gainesville, FL
 Emil Bozin - East Lansing, MI
 Eric Bruton - St. Louis, MO
 Chris Cooper - Worcester, MA
 Lu Deng - Athens, GA
 Aaron Dossey -Gainesville, FL
 David Duda - Gainesville, FL
 Eric Elisabeth - Manhattan, KS
 Tristan Fiedler - Miami, FL
 Jose Gavira - Huntsville, AL
 Oksana Gerlits - Buffalo, NY
 Michael Godsey - Portland, OR
 Jeff Habel - Athens, GA
 F. Hernandez - Buffalo NY
 Andrey Kovalevsky - Buffalo NY
 Sergey Kriminski - Ithaca, NY
 Chris Lehmann - Rockville, MD
 Brock Levin - Manhattan, KS
 Jingzhi Li - Birmingham, AL
 Xue Li - Buffalo, NY
 Zhi-Jie Liu - Athens, GA
 Zhiqiang Lu - Fayetteville, AR
 Baoqing Ma - Buffalo, NY
 M. McFerrin - Huntsville, AL
 Matthew Miller - Evanston, IL
 Peter Mueller - Los Angeles, CA
 Sonia Patenaude - Ottawa, Canada
 Xiangyun Qiu - East Lansing, MI
 Ursula Ramirez -Chicago, IL

Robbie Reutzel - Gainesville, FL
 Colin Rodger - St. Louis, MO
 Bernardo Rodrigues - Buffalo, NY
 Nicholas Silvaggi - Storrs, CT
 A. Solodukhin - Charlottesville, VA
 John Swearingen - St. Louis, MO
 Sun Tao - Storrs, CT
 Wolfram Tempel - Athens, GA
 Joaquin Urbina - Manhattan, KS
 William Watson - Denver, CO
 Jeffrey Wilson - Fayetteville, AR

Latin America

Ricardo Aparicio , Brazil
 Alexandre Araujo, Brazil
 Joao Barbosa, Brazil
 Antonio Carlos, Brazil
 Jarvier Ellena, Brazil
 Jose Ricardo Sabino, Brazil
 Sauli Santos, Jr., Brazil
 Manuel Soriano, Mexico

Europe / UK / Middle East / Russia / India

Andreja Bencan, Slovenia
 Siranush Bezirganyan, Armenia
 Hayk Bezirganyan, Armenia
 Ernesto Estevez, Germany
 Howard Harvey, UK

Alla Lebedinskaya, Russia
 Yael Pazy Benhar, Israel
 R. Venkatachalam , India

The travel awards were made possible by the generosity of ACA members and, in part, by the additional support of the following:

Abbott Laboratories
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 Current Opinion in Structural Biology
 Hampton Research Corp.
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 International Centre for Diffraction Data
 Merck Research Laboratories
 Pharmacia Corporation
 Rigaku/MSC, Inc.
 Structural GenomiX, Inc.
 Univ. of Texas at Austin (Dept. of Chemistry & Biochemistry)



ACA Council met with attendees from Latin America. Front row: João Barbosa, Graciela Diaz De Delgado, Ricardo Aparicio, Manuel Soriano-Garcia, Iris Torriani. Middle row: Javier Ellena, Alexandre Araujo, Sauli Santos, Jr., Marcia Evans, Cindy Soriano-Garcia. Back row: David Rose, Federico Martínez-Ramos, Charlie Carter, Lee Brammer, Doug Ohlendorf, Eduardo Castellano, Bill Stallings

News from the CCDC

The Cambridge Structural Database (CSD) Version 5.23 of the CSD was released in April 2002 and contains **257,162 entries**. The next CSD System release will be distributed in November 2002 and annually thereafter.

CSD Data Updates via the Web

From April 2002, CSD data updates will be available for downloading at regular intervals. This will make it possible for subscribers to keep their copy of the CSD more current between each major release of the CSD System. The URL www.ccdc.cam.ac.uk/prods/conquest/updates/ describes this facility.

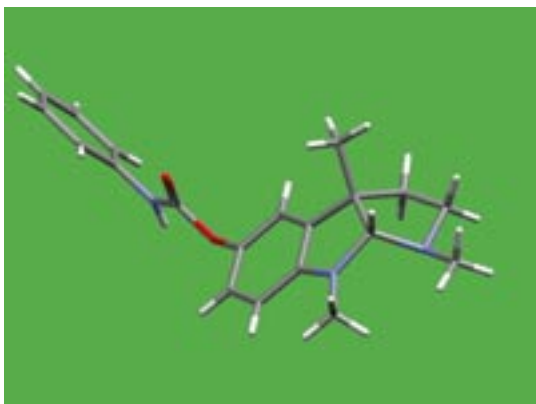
Subscribers will be required to enter their site code and confirmation code in order to download an update. The updates will need to be placed in the same directory as their CSD database files. Within ConQuest 1.4 each update will be shown separately in the View Databases menu. The update packages can be searched either with the main database or separately as desired; this is controlled via options in the ConQuest Search Setup dialogue box.

ConQuest 1.4 (April 2002)

New features include the ability to view the 2D diagram of entries in a floating window when browsing other data categories following a search, and the ability to use a CSD entry as the basis for creating new structure-based queries.

Work on improving the storage and display of data in the CSD has continued with a focus on data associated with deposition. The CIF exported by ConQuest has been extended to optionally allow inclusion of additional text and numeric data items. A 'List' option has been added to PDF output to allow export of, for example, a bibliographic summary of hit entries. For some entries published in IUCr journals, it is now possible to link from ConQuest through to the IUCr's *Crystallography Journals Online* for access to the original article.

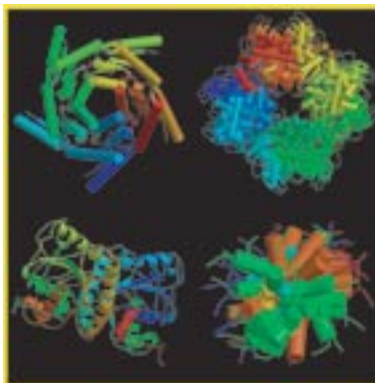
Mercury 1.1 (April 2002)



The Mercury structure visualiser can now read files in MDL mol file and Sdfile formats. These formats do not contain any crystallographic cell or symmetry data, so Mercury cannot display packing diagrams, contact networks, etc. from these files.

Frank Allen

What's on the Cover



Illustrations used in "The Art of Science: Images from the Protein Data Bank". These images were created using MolScript and Raster3D and are available for every structure in the PDB from www.pdb.org/. Graphic design and construction of the cover was done by Christine Zardecki.

Clockwise, from the upper left: **1di0**. Braden, B. C., Velikovskiy, C. A., Cauerhff, A. A., Polikarpov, I., Goldbaum, F. A.: Divergence in Macromolecular Assembly: "X-Ray Crystallographic Structure Analysis of Lumazine Synthase from *Brucella*" (2000) *J.Mol.Biol.*, **297**, 1031; **1rcx**. Taylor, T. C., Andersson, I.: "The structure of the complex between rubisco and its natural substrate ribulose 1,5-bisphosphate" (1997) *J Mol Biol*, **265**, 432; **1hs5**. Davison, T. S., Nie, X., Ma, W., Lin, Y., Kay, C., Benchimol, S., Arrowsmith, C. H.: "Structure and Functionality of a Designed P53 Dimer" (2001) *J.Mol.Biol.*, **307** 605; **1g5p**. Strop, P., Takahara, P. M., Chiu, H. J., Hayley, C., Angove, H. C., Burgess, B. K., Rees, D. C.: "Structure of the All-Ferrous [4Fe-4S]0 Form of the Nitrogenase Iron Protein from *Azotobacter Vinelandii*" (2001) *Biochemistry*, **40**, 651

NSLS con't

and to develop wide-bandgap semiconducting zinc oxide / manganese oxide alloys for UV detectors.

Physicist Eleftherios Iliopoulos, of Boston University, discussed molecular beam epitaxy (MBE) growth of III-V nitride films, particularly alloys of gallium nitride with aluminum nitride and indium nitride.

Finally, materials scientist Karl Ludwig made a brief presentation on behalf of materials scientist Charles Eddy, from the Naval Research Laboratory (NRL) in Washington, DC, who was unable to attend the workshop. Eddy reviewed plasma processing and showed that, while much has been learned about the chemistry of the plasma and the gas above the processed surface, relatively little is known about the actual structure of the surface itself. In this case, as in many examples presented throughout the workshop, the new real-time facilities being planned at the NSLS would provide many opportunities for enhancing our understanding of fundamental materials processes.

Other workshops which took place included one which focused on x-ray sources for studies of ultrafast processes (organized by John Sutherland of BNL), another which focused on EXAFS studies of nanoscale and nanostructured materials (organized by Vincent Harris of NRL), and another which focused on advanced detectors development (organized by Peter Siddons of NSLS).

Patrice Pages

(edited from the original for the ACA Newsletter by Lonny Berman)

**AMERICAN CRYSTALLOGRAPHIC ASSOCIATION, INC.
BALANCE SHEET
December 31, 2000 and 2001**

	CURRENT FUNDS		TOTAL	
	Unrestricted	Restricted*	All Funds	
			2001	2000
ASSETS				
Current Assets:				
Cash	58,702		58,702	47,344
Investments	430,533	335,743	766,296	818,538
Inventory	3,600		3,600	0
Total Current Assets	492,855	335,743	828,598	865,882
Fixed Assets:				
Computers and Printers	6,500		6,500	15,969
Office Equipment	1,300		1,300	3,194
Accumulated Depreciation	0		0	-19,163
Total Fixed Assets	7,800		7,800	0
TOTAL ASSETS	500,655	335,743	836,398	865,882
LIABILITIES & FUND BALANCE				
Liabilities:				
Deferred Dues Income				58,260
Total Liabilities	0		0	58,260
Fund Balance:				
Unrestricted	500,655		500,655	464,284
Restricted		335,743	335,743	343,338
Total Fund Balance	500,655	335,743	836,398	807,622
TOTAL LIABILITIES & FUND BALANCE	500,655	335,743	836,398	865,882

* Current Balances in individual restricted funds
- as of December 31, 2001

Buerger Award	34,621
Etter Award	61,075
Fankuchen Award	64,186
Patterson Award	36,323
Pauling Award	31,526
Supper Award	10,523
Trueblood Award	22,358
Warren Award	27,807
Wood Science Writing Award	47,324

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

We gratefully acknowledge the continued support of ACA CORPORATE MEMBERS

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www.adsc-xray.com

ATPS Inc.
www.atpsinc.com

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Hannover, Germany

Blake Industries, Inc.
blake4xray@worldnet.att.net

Bruker/Nonius
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Cambridge Crystallographic Data Centre
www.ccdc.cam.ac.uk

Charles Supper Company, Inc.
www.supper.com

Compaq Computer Corp.
www.compaq.com

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www.cryoindustries.com

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www.gilson.com

Hampton Research
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International Centre for Diffraction
Data
www.icdd.com

MAR USA, Inc.
www.mar-usa.com

Microsource
www.bede.com/micro.html

Molecular Dimensions, Inc.
www.moleculardimensions.com

MXI Systems, Inc.
www.mxisystems.com

Neuro Probe, Inc.
www.neuroprobe.com

Oxford Cryosystems
www.oxfordcryosystems.com

Oxford Diffraction, Ltd
www.oxford-diffraction.com

Oxford Instruments Inc.
www.oxford-instruments.com

Protein Data Bank
www.rcsb.org/pdb

Protein Solutions
www.protein-solutions.com

Rigaku/MSD, Inc.
www.RigakuMSD.com

Rigaku /Osmic, Inc.
www.osmic.com

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Oviedo, Spain

Wyatt Technology Corp.
www.wyatt.com

X-Ray Research GmbH
www.marresearch.com

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.**

The most up-to-date listings are on the ACA Home Page under the Positions Vacant heading: www.hwi.buffalo.edu/ACA/

Postdoctoral - Protein Crystallographer

There is an opening for a postdoctoral position in protein structure determination and analysis. Applicants with experience in biological X-ray crystallography, protein expression, and purification can send a C.V., and addresses of three references to Dr. Narendra Narayana, Dept. of Biochemistry, Case Western Reserve University, Cleveland, OH 44106. E-mail: nxn17@po.cwru.edu

Positions Previously Listed

Crystallographer-FT/PT

An excellent opportunity to become a team player with an emerging commercial biotech company and work with new drug development crystallization technologies never before available. We are seeking a highly motivated macromolecular crystallographer with 0-2 years of postdoctoral experience who is interested in making a transition from academia to industry. Must have demonstrated productivity and publication record. Strong background in the practical aspects of macromolecular crystallography, including crystallization, data acquisition, structure solution (molecular replacement and isomorphous replacement techniques) and refinement. Experience with membrane bound proteins a plus. Company located in suburban Maryland outside of D.C. Forward Resume to: Shirley Arnowitz, COO, BSI Proteomics, email: shirley@bsiproteomics.com. Fax: 301.990.6487.

ACA 2003 - July 26-31, 2003
Northern Kentucky Convention Center
-Covington, KY



Workshops Topics:

Using the Crystals & Rotax Suite of Programs for
 Chemical Crystallography
 Using the CCP4 Suite of Programs for Macromolecular
 Crystallography
 Cambridge Structural Database
 Crystallization Techniques & Secrets

Buerger Award Symposium: Neutron Diffraction
 (co-organizers: Gerry Bunick & Leif Hanson)

Warren Award Symposium: Time-Resolved Crystallography
 (co-organizers: Phil Coppens & Keith Moffat)

SIG Sponsored Session Topics:

Incommensurate Structures, Membrane Proteins, Dynamics
 of Macromolecules, Important Structural Science in Chemical
 Crystallography and Problem Structures Encountered, New
 and High Resolution Macromolecular Structures, High-Energy
 Materials, Small Angle Scattering Instrumentation, Service
 Crystallography Laboratory Practices, Hard & Soft Materials,
 Grant Writing & Interviewing Skills, Genomics

AACG Sponsored Session Topics:

Crystal Growth Solutions & Techniques, Nucleation



*Local Chair: Bobby Barnett (barnett@pgl.com),
 Program Chair: Jeanette Krause Bauer (jeanette.krause@uc.edu).*

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ACA 2004 - July 17-22, 2004
Chicago Hyatt, Chicago, Illinois



LOCAL CHAIRS



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Chicago skyline downloaded from www.krohn.org with the permission of the photographer, Patrick Krohn, copyright 2001.

60th Pittsburgh Diffraction Conference -Thursday through Saturday, October 3-5, 2002 -Holiday Inn-University Center, Pittsburgh, PA

Symposia:

Thursday:	Neutron Diffraction (organizer: Bryan Craven)
Friday :	Crystallization Issues (organizer: John Rose)
Saturday:	Membrane Proteins & Prions (organizer: Tim Umland) "Protein Crystallography—Twixt Form and Function" (in honor of Martin Sax)

Awards:

Chung Soo Yoo Award: (\$200.00 for the best poster by a graduate student. This award is made in memory of Dr. Chung Soo Yoo who was a research associate in the Department of Crystallography at Pittsburgh when he was killed in the Korean Airlines flight 007 disaster in 1983).

Sidhu Award: (\$500.00 for the best contribution to crystallography or diffraction by an investigator who obtained a Ph.D. after September 1997. This award is made in memory of Professor Surhain Sidhu who was a founding member of the Pittsburgh Diffraction Society. Nominations should consist of 2 copies of the candidate's CV and sponsoring letter(s) and should be sent to Bill Duax, Hauptman Woodward MRI, 73 High Street, Buffalo, NY 14203-1196, FAX: 716-852-4846)

Deadlines:

<i>Abstracts:</i>	<i>September 3</i>
<i>Early Registration:</i>	<i>September 3</i>
<i>Housing:</i>	<i>September 12</i>

More details will be posted on the Pittsburgh Diffraction Conference web site at

www.che.uc.edu/Chemistry/PDC/Pdc.htm

Conference Chair: G. David Smith gdsmith@sauron.psf.sickkids.on.ca

Meeting Calendar

AUGUST 2002

- 4-6 Crystal Chemistry of New Materials & Soft Matter Studied by Synchrotron & Neutron Diffraction. ESRF-ILL Grenoble are organizing this satellite meeting preceding the main IUCr-Geneva Congress.
- 4-6 Neutron and Synchrotron X-Ray Scattering in Condensed- Matter Research (NSCmr2002). Paul Scherrer Institut, Villigen, Switzerland.
- 6-15 IUCr XIX - Congress and General Assembly of the IUCr , Geneva, Switzerland. Joel Bernstein, Chair, Organizing Committee, yoel@bgumail.bgu.ac.il; Menahem Kafory, Chair, Program Committee, kafory@techunix.technion.ac.il. www.iucr@kenes.com/iucr/ and www.geneva-tourism.ch
- 22-26 International Workshop on Photoionization, Hyogo, Japan.
- 25-29 12th International Conference on Small Angle Scattering, Venice, Italy.
- 29-31 The forth international congress "Natural glasses : glasses in geosciences, environmental sciences and archeometry, Lyon, France.

SEPTEMBER 2002

- 4-6 Synchrotron Radiation in Polymer Science II, Sheffield, UK. Sponsored by the European Physical Society, Macromolecular Group.
- 4-7 6th International Conference on Quasielastic Neutron Scattering, Potsdam (near Berlin), Germany.
- 8-12 Chemistry towards Biology, Portoroz, Slovenia. Organized by the Slovenian Chemical Society with the sponsorship of the Federation of European Chemical Societies.
- 10-14 XTOP 2002 6th biennial conference on High Resolution X-Ray diffraction and Topography, Grenoble-Aussois, France.

OCTOBER 2002

- 3-5 60th Pittsburgh Diffraction Conference, Holiday Inn - University Center, Pittsburgh, PA. www.che.uc.edu/Chemistry/PDC/Pdc.htm
- 7-9 29th Annual Stanford Synchrotron Radiation Laboratory Users' Meeting, Menlo Park, CA.
- 10-12 2002 ALS Users Meeting, Berkeley, CA

- 11 35th Annual SRC Users Meeting, Stoughton, WI

- 10 -13 ISGO International Conference on Structural Genomics, Berlin, Germany. www.proteinstrukturfabrik.de/ICSG2002/

NOVEMBER 2002

- 4 - 6 4th NOBUGS Conference, National Institute of Standards and Technology, Gaithersburg, MD, webster.nsnr.nist.gov/events/nobugs2002/.

DECEMBER 2002

- 8- 12 2nd Pharmaceutical Powder X-ray Diffraction symposium PPXR-2, Concordville, PA, www.icdd.com/ppxrd

JUNE 2003

- 4-15 High Pressure Crystallography. Erice, Italy.

JULY 2003

- 21-26 Aperiodic-2003, Belo Horizonte, Brazil.
- 26-31 ACA 2003, Cincinnati, Ohio.

AUGUST 2003

- 10-13 AsCA'03/Crystal-23, Cable Beach Club resort, Broome, Western Australia.
- 14-15 Workshop on Biological Structure , Cable Beach Club resort, Broome, Western Australia.
- 14-19 Sagamore Meeting run by the IUCr Commission on Charge, Spin and Momentum Densities, Cable Beach Club resort, Broome, Western Australia.
- 24-30 21st European Crystallographic Meeting, Durban, South Africa

SEPTEMBER 2003

- 2-6 ECNS 2003 European Conference on Neutron Scattering, Montpellier, France. Contact: R. Vacher, CNRS-SPM, Montpellier, rene@ldv.univ-montp2.fr; tel: 33 4 67 14 34 49; fax: 33 4 67 14 34 98.

JUNE 2004

- 10-21 Polymorphism : Solvates and Phase Relationships. Erice, Italy.

For a more complete list of meeting announcements go to the meetings section of the IUCr website: www.iucr.org or through the US mirror site: iucr.sdsc.edu/iucr-top/

Donald Tuomi, 81, Former ACA Member



Donald Tuomi was a staff member of the Manhattan Project. During World War II, he was involved at the SAM Laboratories at Columbia University's Schermerhorn Building with the successful development of the barrier for the Oak Ridge diffusion plant, which then led to the first atomic bomb using Uranium 235. He earned a BS in Chemistry in 1943 at Ohio State and a Ph.D. in physical chemistry in 1953.

He retired in 1983 from the Roy C. Ingersoll Research Center, Borg-Warner Corporation, with the rank of senior scientist. While there, he was involved in research on thermoelectric energy conservation alloys and the origins of high impact strength in ABS polymers and related materials. In earlier years at the MIT Lincoln Lab, he was involved in the question of oxygen contamination of Ge and Si in collaboration with Homer Priest. During his graduate school years he explored the chemistry details of the Ag-Cs-O S-1 Photocathode used in infrared night vision while working on his dissertation on the crystal structure of Li trichloroacetate. His undergraduate and graduate research led to lifelong interests in relating solid state materials structure to physical properties and synthesis processes as consequences of mass and charge transport through interphases.

He received the Battery Division Research Award from the Electrochemical Soc. In 1973, and the Chicago Technical Society Award of Merit for outstanding technical achievements, service to science, his fellow scientists, and to the community.

Mary Toumi Hammond