AMERICAN CRYSTALLOGRAPHIC ASSOCIATION

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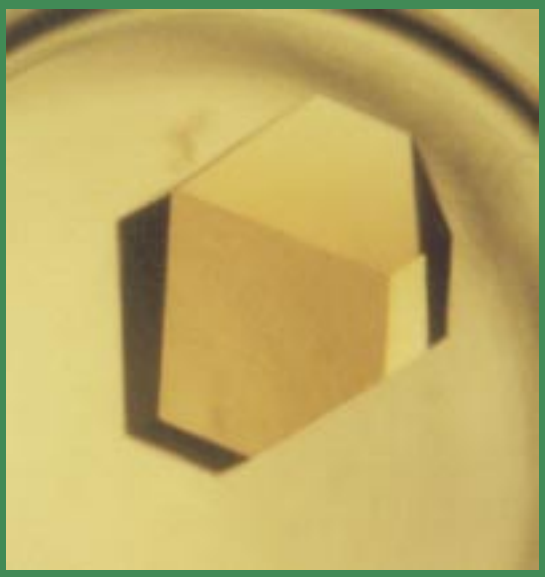

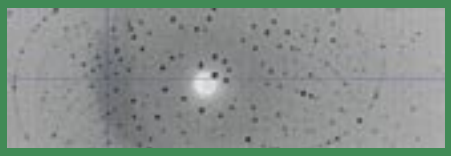

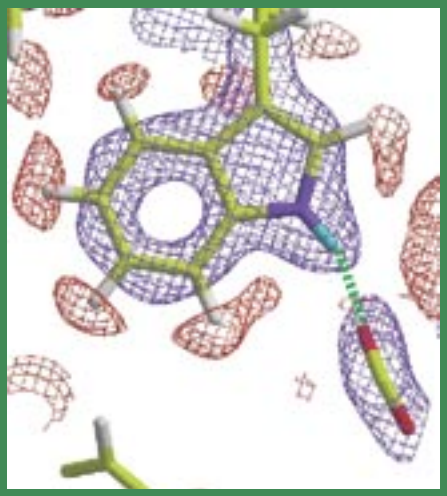

Biological Neutron Diffraction
ACA July 2003

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President's Column

My term as ACA president draws quickly to a close! It is appropriate at such a time to summarize some general thoughts about general status and future directions of the ACA. The ACA Council met Saturday, 9 November in Washington, and most of these remarks derive from discussions at that meeting.

The burst financial bubble has affected everybody, organizations as well as individuals. While we are still in a relatively fortunate financial position, the Council decided to take protective action with our investments, and we have had to come to grips with related realities posed by our operating budget. The most important of these is that costs of our annual meetings have both evolved and grown. Rao pointed out that on a per participant basis, we are subsidizing attendance by an average of nearly $100 per person. These subsidies affect several different areas, but most notably arise from the increasing fee waivers for speakers, AV rental costs for multiple parallel sessions, and, believe it or not, coffee, pastries and cookies provided at breaks. Council weighed these costs carefully, while considering possible increases in registration fees. We can expect compromises as we navigate between Scylla and Charybdis.

The intellectual demographics of ACA special interest groups are the core of the ACA, and they continue to evolve. The Council approved the creation, spurred by Abe Clearfield (Texas A&M), of a new SIG devoted to structure determination by powder diffraction. We expect soon to do the same for an Electron Crystallography SIG organized by Jian-min (Jim) Zuo (University of Illinois, Champagne Urbana). These two areas represent significant colonization by the ACA of new areas with vital intellectual energy. Notably, too, both new SIGs serve important areas distinct from, without excluding, macromolecular crystallography. They therefore will help preserve balance within the community. Both new SIGs evolved from symposia organized at the San Antonio annual meeting. A corollary benefit of these symposia is their effective mentorship role for recipients of the ACA awards, providing a conduit for the enthusiasm and intellectual life of our elder statespersons to successive generations. The program for the Cincinnati meeting promises to continue this evolution, with small molecule and diffraction physics award symposia.

Andy Howard joined us in Washington to update us on plans for the ACA summer school, to be held between 11-26 July at the Illinois Institute of Technology and the APS. Andy's syllabus is fully developed, and we look forward to an outstanding course.

The American Crystallographic community now has strong international representation. Bill Duax began his term as President of the IUCr by visiting countries and regions such as Moldova and Algeria. He finds that the excitement of crystallography has

taken root and will thrive with proper encouragement. Among the innovations he has suggested for the ACA is that we entertain memberships from nations with their own crystallographic associations, but whose citizens are ill equipped to subscribe as individuals. Our initiative, with the US National Committee for Crystallography, to foster the growth of Latin and South American participation in the ACA could benefit from this type of national membership. Such action would require a change in the ACA bylaws, and this question will be taken up at the annual business meeting next summer in Covington. Please think about it, and come to the meeting prepared to discuss it.

While I'm encouraging you to action, it is appropriate to urge you to spread the word about the benefits of membership to non-ACA members. Council members have not decided on a formal drive, but recognize that we number about the same today as we did five years ago. Crystallography has certainly grown substantially in that period, so we are not keeping up. Ask your colleagues why they are not ACA members, and urge them to attend the 2003 meeting to see why membership is so worthwhile. After a year at the helm, I can tell you that service to the ACA is an unqualified positive experience whose best reward is working with such wonderful people. I am grateful for the opportunity you have given me.

Charlie Carter

Guest Editorial: IUCr President William Duax

It is a pleasure and an honor to have been elected to serve the crystallographic community as President of the International Union of Crystallography (IUCr). I want to thank ACA Council Members past and present, the members of the US National Committee for Crystallography and all members of the ACA for the support they have given me in the past. I also want to ask for your continued help with the challenges ahead.

The US crystallographic community was a key player in the founding of the Union and US crystallographers have served the Union consistently as editors and co-editors of Union Publications and as members of all IUCr Commissions. The US has hosted the IUCr Congress twice and past presidents have included Phillip Coppens and Jerome Karle.

Now, more than at any other time in history, it is important that we set aside national interests and embrace the principles of the International Union. Those principles include free circulation of scientists, education of the new generation of scientists everywhere, and assistance to emerging nations. Emerging nations can benefit from the use of the powerful techniques of X-ray crystallography in order to analyze, understand and use the unique natural resources within their countries whether mineralogical, chemical, or biological in nature.

It is noteworthy that the Union consistently uses its financial resources to support countries in need and students everywhere. I urge you to support all of the activities of the IUCr. Consider publishing some of your best work in Acta or starting a personal subscription to an *Acta* Journal (ACA members may subscribe to *Acta E* at a reduced rate). Establish a collaboration with a research scientist on another continent in order to advance science and support international communication. Consider volunteering to assist one of the Commissions of the Union in achieving its objectives. If you have ideas, concerns or opinions about the activities of a Commission of the Union, please express them. If you think that there are areas vital to crystallography and crystallographers that might be served by a new commission, a new publication, or a new volume of the International Tables, address your ideas to me or the individuals you consider best qualified to evaluate and implement your requests.

The Regional Affiliates of the IUCr have become powerful resources to advance the goals and principles of the Union. In 1993 the members of the ACA responded to the needs of our colleagues in Russia. Today the ACA is sensitive to problems in Latin America. I applaud the ACA's Latin American initiative that is based upon asking your neighbors to the South how you can work with them to achieve their goals, rather than setting goals for them. The European Crystallographic Association has a vital African Initiation and the more advanced countries in the Asian Crystallographic Association are helping to strengthen crystallography in their region. When you travel to another country, consider yourself an ambassador for crystallography. Contact crystallographers in the cities you visit and find out what they are doing and, where appropriate and feasible, offer your support and assistance. This is especially important if you visit a country that is not now a member of the Union.

Carolyn, Sarah and Bill Duax at the banquet in Geneva

Perhaps the best thing each of you could do for yourself, your science and others would be to volunteer for a leadership role in a scientific organization, work for international cooperation, and encourage young people to become involved.

Bill Duax

News from Canada: November, 2002

1. ***The Canadian National Committee*** is scheduled to meet on December14th in Montreal. The Committee currently consists of Suzanne Fortier (Chair), Joe Schrag (Secretary), J.P. Charland, Stan Cameron, Frank Hawthorne, Francois Brisse and David Rose.

2. ***Student Travel Awards*** to the IUCr meeting in Geneva were granted to **Ning Wu** (E. Pai lab) and Lili Sampaleanu (L. Howell lab).

3. ***New laboratories:***

Thanks to funding opportunities from the Federal Government as well as some of the Provinces, several new (or relocated) laboratories have been initiated. A selection (probably not exhaustive) of these includes: Marie Fraser and Kenneth Ng at the University of Calgary, Frederic Pio and Mark Paetzel at Simon Fraser University (Vancouver), Steven Mosimann at the University of Lethbridge, Alberta, Albert Berghuis at McGill University, Montreal, Murray Junop at McMaster University, Dinesh Christendat at the University of Toronto. There are recruitment efforts continuing at several Universities across Canada.

4. ***Buffalo/Hamilton/Toronto Regional Crystallography***

Every year, crystallography groups from the Niagara region gather for a one-day symposium at McMaster University in Hamilton. Traditionally, the meeting is termed the BHT after the founding centres. However, in recent years we have had participation from Rochester, London and even Kingston (a heroic 4 hour drive each way). The meeting follows the format of a morning session by an invited speaker of international standing in a (technical) area of crystallography, to describe in a workshop format some of the most important recent advances. The afternoon is devoted to short talks by trainees from the participating groups. In past years, our expert visitors have included Jim Pflugrath, Alex McPherson, Axel Brunger, Wayne Hendrickson, B.C. Wang and other distinguished colleagues. The visitor delivers a PENCE research seminar (see item 5) on the day before the meeting in Toronto. This year's meeting was held on November 1st and the visiting presenter was Gerard Kleywegt, on "Structure Validation".

The meeting has been supported by contributions from our friends at PENCE, Hampton Research, Molecular Structure Corporation and Emerald Biosciences. Anyone who wants to make the trip to Hamilton is welcome to join us for future meetings.

5. ***CanadaQuirks: PENCE***

In this item, your correspondent will attempt to clarify Canadian terms, organizations, issues, etc. that might be of interest to the Crystallographic community.

The Networks of Centres of Excellence program (NCE) is a funding initiative created by the Federal government about 12 years ago. The concept of the program was to create virtual Centres of collaboration among researchers working in a priority area, in order to foster interactions across the country. There have been 2 or 3 rounds of NCE funding in areas as diverse as Stem Cell Research, Bacterial Diseases and Materials Science.

The NCE most concerned with Structural work is PENCE, the Protein Engineering NCE. One of the initial NCE's funded, PENCE now includes as members many of the macromolecular crystallographers in Canada, as well as workers in other areas of Protein Science in the most general sense. PENCE participates in communication and educational efforts among the participating institutions, for example by sponsoring seminar programs across the country. There is also a commercialization aspect to the NCE's with several industrial participants and spin-off companies. For more information, vis ***www.pence.ca***.

Any contributions to future Canadian reports are welcome to ***drose@uhnres.utoronto.ca***. News from outside your correspondent's geographical and/or technical areas is especially welcome.

David Rose

Workshops Developed in Cooperation with the American Physical Society and the Brazilian National Synchrotron Light Laboratory

LNLS, the Brazilian National Synchrotron Light Laboratory, is hosting an Interamerican Workshop on Synchrotron Radiation and Applications to Macromolecules and Biological Systems, December 9-11, 2002, in Campinas, São Paulo, Brazil. The LNLS began operations in July 1997. At present, eleven beamlines are in operation for research in VUV and X-ray spectroscopy, small angle X-ray scattering, X-ray fluorescence, X-ray diffractometry, deep lithography, and protein crystallography. The light source, a 1.37 GeV electron storage ring, is particularly well suited for VUV and soft X-ray experiments, although bending magnet radiation in the 10 keV region is also regularly used.

LNLS is located on a pleasant campus close to UNICAMP (State University of Campinas). Campinas is located 90 km from the city of São Paulo and can be reached by direct flights from Rio de Janeiro, Belo Horizonte, São Paulo, and other Brazilian cities. Frequent bus services link Campinas and São Paulo and also Campinas and São Paulo International Airport (GRU).

The workshop will be short, focused on research in specific areas of synchrotron applications to macromolecules and biological systems. In addition to plenary colloquia the workshop will have oral and poster presentations on the following topics:

Crystallographic structure of proteins

Protein-lipid interactions

Macromolecular assemblies

Biocompatible polymers

Polymeric drug carriers

Biocomposites

Speakers from the US and Europe will include: ***Ana Gonzalez*** and ***Sebastian Doniach*** (SLAC), ***Phil Bourne*** (UCSD), ***Paul Russo, Britt Thomas*** and ***Vincent Licata*** (LSU), ***Vivian Cody***

(HWI), ***William Shepard*** (ESRF), ***Bob Sweet*** (BNL), ***Sol Gruner*** (Cornell), ***José Onuchic*** (UCSD), ***Benjamin Chu*** (SUNY), ***Marv Hackert*** (UT at Austin), ***Rodouane Borsali*** (Université de Bordeaux) and ***Angel Garcia*** (Los Alamos). Speakers from Brazil will include: ***Igor Polikarpov*** and ***Glaucius Oliva*** (Universidade de São Paulo) , ***Jerson Lima*** and ***Sérgio Ferreira*** (Universidade Federal de Rio de Janeiro), ***Watson Loh*** (Universidade Estadual de Campinas), ***Dario Grattapaglia*** (Cenargen-Embrapa), ***César Chagas*** (Instituto Biológico- São Paulo) and ***Wim Maurits Degrave*** (Fundação Oswaldo Cruz- Fiocruz).

The meeting will be reviewed in the Spring Newsletter.

Iris Torriani

Jürg Waser (1916- 2002)

Jürg Waser, who was president of the ACA from 1960 to 1961 (vice-president, 1959-1960), died at his home in La Jolla on August 16,2002 at the age of 86. He is survived by his wife Plüdi, children Nicki, Peter and Kathy, grandson Andrew Waser, and stepson Roy Weiss.

Jürg was born in Zurich and attended the University of Zurich. He went to Caltech on a one-year graduate exchange program in 1939 but remained because of World War II, receiving his PhD (chemistry) in 1944 under the supervision of Linus Pauling. He continued at Caltech as an Instructor in Mathematics and a Research Fellow in Chemistry until 1948, when he returned to the University of Zurich. He soon came back to the United States as Professor of Chemistry at Rice University in Houston, and returned to Caltech as Professor of Chemistry in 1958. He retired in 1975.

Jürg's primary responsibility at Caltech was to teach the introductory chemistry course required of essentially all undergraduates. He taught it meticulously; meticulous in his preparations for lectures, meticulous in his insistence that he thoroughly understand the subjects himself, meticulous in his supervision of the Teaching Assistants. He was famous for his "pop qwisses" (pronounced with his native Swiss accent), and for his stern yet sympathetic mien. In effect, he ruled the course with an iron hand - well hidden under a soft glove, for he was always willing to give help to any student who sought it. When he could find no satisfactory textbook for the Analytical Chemistry portion of the laboratory work, he wrote one; it went through two editions and was used in several other colleges. He also wrote a slim volume on "Basic Chemical Thermodynamics", to help the students (and TA's) understand these concepts. His thoughtful lectures and his close interaction with his Teaching Assistants surely inspired many students, both undergraduate and graduate, to become more disciplined and more understanding - as well as far more knowledgeable in their pursuit of a scientific career.

Although most of his time at Caltech was spent with his teaching duties, he carried out extensive research in the field of structural chemistry, using the experimental methods of x-ray diffraction and his thorough knowledge of mathematics; he particularly enjoyed the concepts and notations of dyadics. He was one of the first to include "restraints" in the least-squares refinement process. After his retirement he turned more and more to questions involving basic thermodynamics, and often collaborated on this subject with his close friend, the late Verner Schomaker (also a past president of the ACA) and with Hans Kuhn of the Max Planck Institut at Goettingen, Germany on theories concerning the origin of life.

Jürg was tall and stately, and an excellent dancer - particularly enjoying Viennese waltzes. He also enjoyed camping and the outdoors. He returned to Switzerland most summers, and it is easy to visualize him striding along with an alpenstock and a red-feathered hat, planning in his mind a lecture on chemical equilibrium.

Dick Marsh

William Glenn Sly (1922-2002)

William G. Sly, professor emeritus of chemistry, Harvey Mudd College, died on September 9, 2002. He was born on June 15, 1922, in Arcata, California. He attended San Diego State University, where he received a bachelor's degree in Chemistry. Bill went on to receive a doctoral degree from Caltech in 1955, followed by postdoctoral study with David Shoemaker at MIT. He joined the faculty at Harvey Mudd College in 1958.

Bill's graduate advisor at Caltech was Holmes Sturdivant, and he worked closely with Dick Marsh, Verner Schomaker, and others at Caltech in the early 1950's on x-ray diffraction. While he did not publish a large number of structures in his career, what he did work on was timely, interesting, and difficult. His thesis focused on the structures of β-carotenes, and principally on the three-dimensional structure determination of 15,15'-dehydro-β-carotene–a formidable and very interesting molecule at the time because it contained a long *trans* chain of alternating single and double bonds. Following that, he reported on a redetermination of the structure of $KBrF_4$, and "Marshed" an earlier report of the structure. He also determined the structure of dicobalt hexacarbonyl diphenylacetylene, which was one of the first organometallic compounds with a metal-metal bond. At MIT he worked with David Shoemaker on programming the new IBM 704, with improvements on 3D Fourier and Patterson map calculations, based upon Schomaker's "M-card" system at Caltech (on the IBM 402 tabulator and sorter). In addition, he focused on two very interesting structures: cyclooctatetraenecarboxylic acid (from Arthur Cope's lab) to ascertain the shape of the molecule and bonding details, and on the R-phase of the ternary compound Mo-Co-Cr, with a comparison to the σ, δ, and P-phase structures.

Bill began teaching at Harvey Mudd College in 1958, retired in 1992, and continued to teach laboratory courses part time. His tenure of 34 years was at the time the second longest in college history. Bill's teaching and research interests were in physical chemistry. He was referred to as "Wild Bill" and as "The Snowman" for the amount of information he presented in his courses. He set and maintained the college record of filling seventeen boards during a fifty-minute PChem lecture, often without the use of any notes. Though formidable in his lecturing style, Bill was completely

approachable one-on-one. He possessed a wide range of diverse skills–glassblower, instrument maker, and electronics whiz–that were of invaluable use in designing laboratory experiments; undoubtedly skills acquired from his early days at Caltech while working for Sturdivant. Many of the PChem lab experiments that he designed over thirty years ago are still in active use. He loved crystallography, and followed the advances in the field intermittently. He worked with Joe Kraut's group at UCSD on sabbatical in the late 1970's, and later worked with me at Caltech on the structure of an organometallic photolysis product. When I gave a seminar at HMC earlier this year on microcrystallization and advances in structural genomics, he had a number of questions afterwards.

In addition to his rigor and love of science, Bill was an avid sportsman. He enjoyed tennis and softball, as well as fishing, camping, and skiing. Legend has it that he once fielded first base in a softball game at Caltech with a full, hard leg cast (his leg broken from a skiing accident); fortunately, when he made a hit, the other team let him use a pinch runner. He seemed to fold sports, science, and other interests together easily. As an example, to complete the requirements for a graduate degree, Caltech students would typically prepare and defend a few research proposals after presenting their dissertation to the faculty. Not surprisingly, one of Bill's proposals was a detailed plan on how to improve the Caltech Chemistry softball team. At HMC, he was critically important in the development and nurture of the athletics program, and Bill was well-known throughout Southern California for his participation in SCIAC (Southern California Intercollegiate Athletic Conference). He also designed and installed the first sound system in Ducey Gym. He was a dedicated Dodgers fan. It was not unusual to find him in the lab or his office working with the broadcast in the background.

An early letter of recommendation stated that he was a "diamond in the rough." He was, indeed, multi-faceted, brilliant, sharp, and tough without the polish. His students, colleagues, friends, and family will all miss his friendship, intellect, energy, and support.

Bernie Santarsiero

The Gregori Aminoff Prize in Crystallography

The Royal Swedish Academy of Sciences has awarded the prize for 2002 to **Meir Lahav** and **Leslie Leiserowitz** from the Department of Materials and Interfaces, Weizmann Institute of Science, Rehovot, Israel, for their fundamental studies of crystal growth and application to separation of enantiomers and for their studies of surface structures by synchrotron radiation. The prize was presented at the ordinary meeting of the Academy 11th September.

Lecturers at the Aminoff symposium: Left to right: Ivar Olovsson (organizer), Michael Ward, Meir Lahav, Jack Dunitz, Angelo Gavezzotti, Lia Addadi, Leslie Leiserowitz, Jens Als-Nielsen, Michael McBride, Stephen Byrn.

A symposium on the theme '*Crystal Growth and Surfaces'* was arranged the following two days. The following lectures were delivered:

Meir Lahav, Weizmann Inst: *Shaping crystals with 'tailor-made' auxiliaries;* **Lia Addadi**, Weizmann Inst: *Chirality at the interface between crystals and biology;* **Michael Ward**, Univ of Minnesota: *Crystal growth interfaces: Visualization and controlled nucleation;* **Michael McBride**, Yale : *Crystal growth and dissolution near equilibrium: Direct observation by atomic force microscopy;* **Stephen Byrn**, Purdue University: *Crystallization and solid state chemistry of pharmaceutical compounds;* **Jack Dunitz**, ETH Zürich: *Polymorphism: The same yet different;* **Jens Als-Nielsen**, Niels Bohr Inst: *The physics and use of synchrotron radiation for studying surfaces and interfaces;* **Angelo Gavezzotti,** Univ of Milano: *Understanding crystal nucleation: Can a cheap computer help a million-dollar project?*; **Leslie Leiserowitz**, Weizmann Inst: *Crystalline Architectures at the air-water interface. Relevance to crystal nucleation.*

Ivar Olovsson

Alexander von Humboldt Research Award

Vladimir G. Tsirelson, Professor and Head of the Quantum Chemistry Department at the Mendeleev University, Moscow, has been named as a recipient of the 2002 Alexander von Humboldt Research Award in the field of crystallography. He received the award for his contribution to the development of theoretical principles of accurate x-ray diffraction analysis, methods of accurate measurement, and interpretation of electron density and electrostatic potential. He has also created numerous schemes for calculation of electronic properties of crystalline systems. The remarkable feature of the Prof. Tsirelson's research is that it combines quantum chemical methods and x-ray and electron diffraction experiments. These studies have provided a step towards an essentially new level of knowledge concerning bonding in molecular and crystalline systems. Now Prof. Tsirelson will continue his research in collaboration with Muenchen Technical University, Wuerzburg University and Potsdam University.

The ACA Summer Course in Small Molecule Crystallography.

This course will be offered August 3 - 13, 2003 at the Indiana Univ. of Pennsylvania, in the town of Indiana located about 80 miles east of Pittsburgh. Each day there will be 3 lectures in the morning on single crystal and powder diffraction methods, followed by afternoon and evening workshops for problem solving and for crystal structure determination. Attendees are encouraged to bring their own single crystal or powder samples for X-ray data collection. Attendees are expected to have at least an undergraduate science degree. No prior experience of X-ray crystallography will be assumed, but attendees are advised to read in advance *"Crystal Structure Analysis: A Primer"*, by Jenny P. Glusker and Kenneth N. Trueblood, Oxford Univ. Press (1985).

The organizers aim for a total of 30 attendees, who in past years have come from academia (students and faculty), government and corporate institutions, both in the U.S. and from abroad. Tuition will be $200. Dormitory housing at IUP (including breakfast and lunch) is available for a total of $294. Fifteen graduate student scholarships will be offered. These will consist of a waiver of tuition and dormitory costs. The scholarships will be awarded based on the student's (1) scientific ability, (2) expected benefits from the course and (3) skills in English.

Instruments available will be two Bruker-Nonius single crystal diffactometers (a CAD4 at IUP and a modern instrument with CCD detector located at the University of Pittsburgh which will be electronically linked to the X-ray Lab at IUP). Also available will be a Bruker-Nonius D8 powder diffractometer in the X-ray Lab at IUP. There will be adequate computing facilities including access to the Cambridge structural data base and the ICDD powder diffraction data base.

The lecturers for the course will be **Robert Blessing** (HWI, Buffalo, NY), **Bryan Craven** (IUP; emeritus Univ. of Pittsburgh), **Steven Geib** (Univ. of Pittsburgh), **Charles Lake** (IUP), **David Smith** (Hospital for Sick Children, Toronto; emeritus HWI, Buffalo, NY), **James Stewart** (emeritus Univ. of Maryland), **Patrick Woodward** (Ohio State Univ.) and **John Woolcock** (IUP).

The Course registration form can be obtained from the ACA web site at ***www.hwi.buffalo.edu/ACA/***. Completed forms must be received before June 1, 2003 by Prof. Bryan Craven, Chemistry Department, Indiana University of Pennsylvania, Indiana, PA 15705, USA or electronically by Prof Lake at *lake@grove.iup.edu*. Further information will be updated on the web site or can be obtained from ***craven@icubed.com***.

The organizers of this ACA Course shall observe the basic policy of nondiscrimination and affirm the rights of scientists throughout the world to adhere or to associate with international scientific activity without restrictions based on nationality, race, color, age, religion, political philosophy, ethnic origin, citizenship, language, or sex, in accordance with the Statutes on the International Council of Scientific Unions. At this Course, no barriers will exist which would prevent the participation of bona fide scientists.

Bryan Craven and Charles H. Lake, Organizers.

The ACA Summer Course in Macromolecular Crystallography.

Illinois Institute of Technology (IIT) and the crystallographers of northern Illinois and southern Wisconsin announce an upcoming ACA summer school in macromolecular crystallography. It will be held sometime close to the 2003 ACA meeting (exact dates willl be set shortly) on the campus of Illinois Institute of Technology, on the south side of Chicago near Comiskey Park. The course will include lectures and laboratory sessions at IIT as well as extensive hands-on experiments at several of the Collaborative Access Team beamlines at the Advanced Photon Source (APS), Argonne National Laboratory. APS is the brightest source of X-rays in the US and has several beamlines dedicated to macromolecular and small-molecule crystallography. Discussions are underway to augment the IIT and APS portions of the course with laboratory sessions at other academic crystallographic facilities in northern Illinois. The course will include both small-molecule and macromolecular crystallographic topics, and participating faculty will be drawn from several of the Chicagoland and Wisconsin universities. Students participating in the course will be invited to stay in student housing at IIT for reasonable rates. Funds for the course will be derived from the ACA itself, from the IUCr, and from corporate contributions. IIT is providing space and intellectual resources, as is the APS. For further information contact: Andrew J. Howard, Associate Professor of Biology, IIT, 3101 S. Dearborn St, Chicago IL 60616, phone 312-567-5881, fax 312-567-3576, e-mail ***howard@iit.edu.***

The organizers of this ACA Course shall observe the basic policy of nondiscrimination and affirm the rights of scientists throughout the world to adhere or to associate with international scientific activity without restrictions based on nationality, race, color, age, religion, political philosophy, ethnic origin, citizenship, language, or sex, in accordance with the Statutes on the International Council of Scientific Unions. At this Course, no barriers will exist which would prevent the participation of bona fide scientists.

Andrew Howard

Eisenberg Elected to National Academy

David Eisenberg, professor of biological chemistry and molecular biology, University of California, Los Angeles, and director, UCLA-US Department of Energy Laboratory of Structural Biology & Molecular Medicine was recently elected to the Institute of Medicine, one of the four sister institutions that make up the National Academies.

ACA Continuing Education Committee.

All four members met during the ACA San Antonio Meeting, noting that over the past few years our committee had become rather moribund so that, by default, some of its responsibilities had been taken over by the ACA Council. This includes the review of ACA travel grants to assist students in attending meetings and the review of proposed workshops submitted by the SIG's for forthcoming ACA meetings.

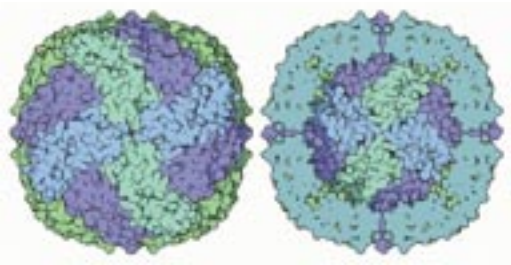
Current members want to reinvigorate the Continuing Education Committee and to resume responsibilities that we were elected to provide. We believe that the Committee should become more effective in advising the ACA Council regarding Continuing Education.

First, we have drafted Guidelines for ACA Workshops which we will submit to the ACA Council. Our members have noted that there seem to be no uniform standards for these workshops. Workshop sessions should not be interchangeable with lectures that are given as part of the scientific sessions of the ACA. Workshops should allow hands-on participation so that attendees can practice their skills. Attendees should fill out evaluations of the workshop to be reviewed by our committee. Workshop organizers should provide the Buffalo ACA office with a summary and with a copy of handouts, CDs or other material used in the workshop.

Second, our committee should have a role in advising the Council about the Summer Courses in Crystallography which have been offered over the past decade and which will resume in the summer of 2003. At the end of the course, the organizers should provide our committee with a summary statement and evaluations gathered from the attendees and should also furnish a statement of their intentions for subsequent years.

Third, our committee should be active in sponsoring sessions at ACA meetings which are related to crystallographic education. While such sessions have been a valuable part of recent meetings, they have been the result of individual initiatives within the SIGs without having the formal endorsement of the ACA as a whole.

Phillip Fanwick, Winnie Wong-Ng, Marilyn Olmstead, and Bryan Craven, Chairman



From the PDB's Molecule of the Month feature by David S. Goodsell. PDB ID 1fha, Lawson, D. M., Artymiuk, P. J., Yewdall, S. J., Smith, J. M., Livingstone, J. C., Treffry, A., Luzzago, A., Levi, S., Arosio, P., Cesareni, G., et al.: Solving the structure of human H ferritin by genetically engineering intermolecular crystal contacts. Nature 349 pp. 541 (1991).

ACA Communications Committee

The activities of the Communications Committee since the Los Angeles ACA Meeting have involved:

1. Redesigned ACA web site.

The Committee participated in the implementation of the redesigned ACA web site. Our involvement consisted of providing design opinions via electronic mail and testing features of the redesigned web site prior to final rollout.

2. Educational Links on the ACA web site.

The Committee continues to interact with Howard Jones, a member of the ICDD. Dr. Jones is heading an effort to upgrade the educational content of and educational links available from the ICDD web site. Our intention is to work jointly to identify useful crystallographic educational web links and materials that are not yet available from either the ACA or ICDD web sites.

3. "Crystallography Web Watch" column in Newsletter.

The Committee continues to author a "Crystallography Web Watch" column for the *ACA Newsletter*. Committee members identify web sites of interest to crystallographers and briefly summarize the content of these sites. Columns have been published in every issue of the *Newsletter* since Fall 2001 Our intention is to continue writing these columns for inclusion in future issues of the *ACA Newsletter*. We urge the ACA membership to help us in this effort by forwarding the addresses of their favorite web sites to the Committee chair.

4. Press kit for Meetings and other ACA uses.

The Committee continues to explore the development of a "press kit" that would contain information about the ACA, scientific advances involving crystallography and details about ACA meetings. One use for the kit would be to publicize the ACA and crystallography to the local press of a meeting's host city, leading to regional, and possibly national, press coverage of this and future meetings.

The majority of our efforts have centered on the Internet and its effective use in crystallographic research and education. We are particularly interested in the ACA web site being kept current and interesting. The Committee is unaware of a formal mechanism to add new links, especially those identified in "Crystallography Web Watch" columns, to the ACA web site. Such a mechanism should be established or better publicized if it is already in place. We can think of no better way to enhance the impact of "Crystallography Web Watch" than to include links identified therein on the ACA web site.

F. J. Rotella, Chairman, J. Sack, J. Krause Bauer, and K. Onan

Crystallography Web Watch

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

Periodic Table online — Webelements is one of the more complete periodic tables available on the web. Selecting an element provides not only the usual information on physical and chemical properties but also the name of the element in seven languages, information on the element's preparation or isolation and links to pages describing compounds of the element and their chemistry (with references). Photographs of the elements and depictions of their atomic and crystal structures are also present, as are some clever cartoons based on the elements and their properties. ***www.webelements.com***

Women in Science — The San Diego Supercomputer Center has an excellent web page giving short biographies of sixteen women who have made significant scientific contributions(***www.sdsc.edu/Publications/ScienceWomen/***). The profiled *Women in Science* include two crystallographers, Dorothy Hodgkin and Rosalind Franklin. Hodgkin's life and career are also profiled in an episode of *The Engines of Our Ingenuity*, a National Public Radio program that tells the story of how our culture is formed by human creativity. A transcript of the episode (#933) is available on the University of Houston's College of Engineering web site(***www.uh.edu/engines/epi933.htm***), as are those of the over 1750 episodes of the program. Biographies of both women can also be found on the web site for the Public Broadcasting System's television series, *A Science Odyssey* (***www.pbs.org/wgbh/aso/databank/***), which details 20th century discoveries and the people who made them.

X-ray Data Booklet online — A web version of the latest edition of the *X-ray Data Booklet* is now available. The booklet, first published in 1987, is a useful compendium of graphs and tables providing data on all things x-ray. The web site is organized like the booklet. Most links download PDF files of sections in the booklet, and tables are available in both HTML and PDF formats. The information provided is particularly useful to those doing experiments at synchrotrons: ***http://xdb.lbl.gov***

MERLOT — A particularly fine web site (and wine, for that matter) is MERLOT, the Multimedia Educational Resource for Learning and Online Teaching. MERLOT is a free and open resource designed primarily for faculty and students of higher education. Copious links to online learning materials in virtually all subject areas are collected there along with annotations such as peer reviews and assignments. In the areas of science and technology alone, MERLOT has over 3000 links, which currently include 460 biology, 186 chemistry, 51 geology and 1434 physics web pages: ***www.merlot.org/Home.po***

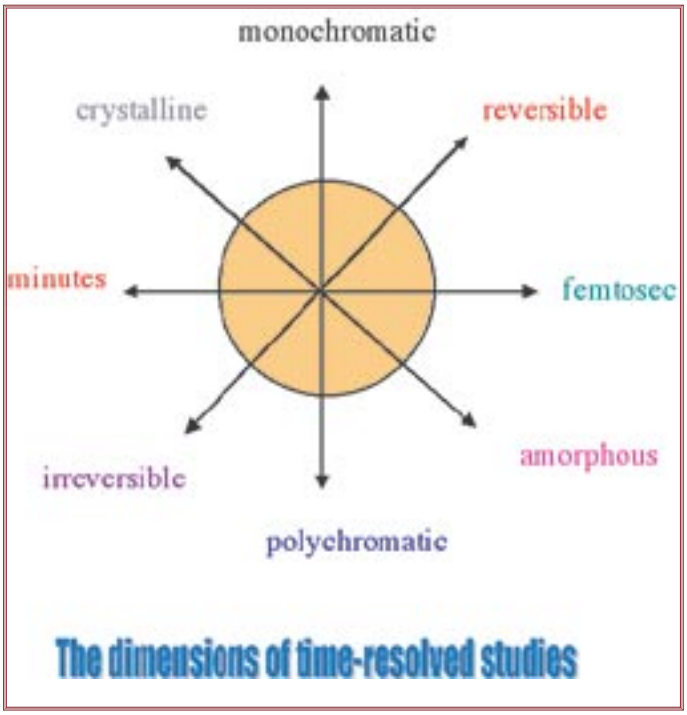
For the Macintosh user — Total Resolution, a US commercial software vendor specializing in scientific software for use in electron microscopy and crystallography, sells two products specifically for the Macintosh. *MacTempas* is high-resolution TEM image simulation software that can calculate and display TEM images and diffraction patterns. The second program, *CrystalKit*, allows crystalline defects of various kinds, from point defects to grain boundaries and precipitates, to be built starting from single crystal data. Both programs can be used in tandem (i.e., output from one can be input to the other): ***www.totalresolution.com/***

Old Source Code — Source code of crystallographic software dating as far back as the 1960's may be downloaded from the Crystallography Source Code Museum. Many *FORTRAN* "golden oldies" may be found there, as well as more recent *C* and *C++* code: ***www.cristal.org/museum***

Calling All Rockhounds — Bob's Rock Shop is an online publication targeting rock collectors, lapidary hobbyists, gemologists, mineralogists and other rockhounds. Of interest to crystallographers is a page by Mike and Darcy Howard explaining crystals, unit cells, symmetry, crystal systems and common habits found in minerals very nicely. Other interesting links include a mineral identification key, the hardness of minerals and rocks and a mineral specimen gallery containing many beautiful photographs: ***www.rockhounds.com/rockshop/table.html#xtal***

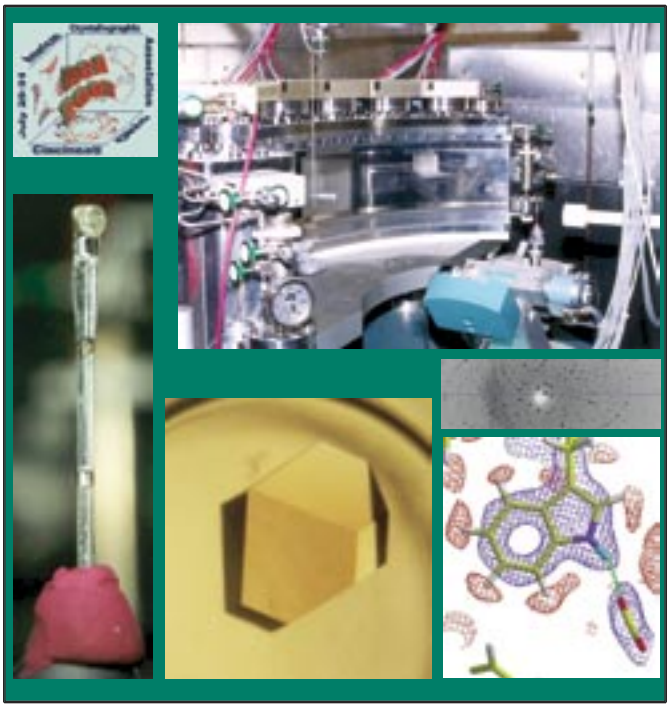
Have a favorite web site that you'd like to see in a future **Crystallography Web Watch** and possibly linked on the ACA web site? If so, send the web address and a short (1 or 2 sentence) description to Frank Rotella (fjrotella@anl.gov)

Frank Rotella.



The 2003 ACA Meeting in Northern Kentucky will include a special symposium on Time-Resolved Crystallography, organized by Phil Coppens and Keith Moffat.

What's on the Cover



Depicted on the cover of this issue are images from recent macromolecular neutron crystallography experiments. The growing interest in neutron crystallography is paralleling the development of dedicated beamlines, new detectors, and new software tools to handle multi-wavelength data. At moderate resolution, neutron diffraction data can provide strong support for the orientation of hydrogen atoms in water molecules, and can elucidate the ionization states of amino acids. Neutron diffraction is unsurpassed as a method for accurately locating the positions of hydrogen atoms, especially the mobile hydrogens needed for determining enzymatic mechanisms, hydrogen bonding patterns, and solvation of macromolecules in enzymes and other macromolecules. (On the bottom right, neutron density of a tryptophan residue from rubredoxin clearly shows the difference between H atoms (red contours) and D atoms (blue contours) (kindly provided by Robert Bau)). The new LANSCE macromolecular neutron beamline at Los Alamos has been commissioned (upper right), providing an opportunity to collect diffraction data from larger proteins such as D-xylose isomerase (middle right, left side), from large crystals grown in hardware developed by NASA for microgravity studies (bottom middle). Topics ranging from structures to new beamlines and proposed new sources will be discussed in this year's Transactions Symposium at ACA 2003. When the next generation of neutron sources such as the Spallation Neutron Source (SNS) become operational in several years, the crystallographic community will benefit from an increase of several orders of magnitude in neutron flux. Neutron scattering and diffraction will soon become more powerful and more widely available tools for macromolecular crystallographers.

Gerry Bunick

ACA Solicits Nominations for a New Award Honoring the late Professor Margaret C. Etter

The ACA is seeking nominations for the new Margaret C. Etter Early Career Award, which will recognize achievement and future potential among those at an early stage in their independent career. The award celebrates Professor Etter's tremendous scientific accomplishments and especially her well-deserved reputation as an outstanding mentor of students and junior colleagues.

Nominations may come from any source, but the ACA is especially interested in input from Chairs of Academic and Industrial departments, because of the potential summarized in the guidelines listed below to recognize outstanding achievement and exceptional potential in crystallographic research demonstrated by a scientist at an early stage of their independent career.

The award honors the memory of 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 ACA 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 PhD degree, not including career breaks, and must have begun their first independent (not post-doctoral) position within the past 6 years. Nominees employed in tenure-track academic positions must not yet have received tenure. Self-nominations are not permitted. Within these guidelines, eligibility should be considered as broadly as possible. Nominees may be employed in regular academic positions, as service crystallographers, in industrial positions, or in government laboratory positions. 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. The original deadline for nominations having passed, we have EXTENDED THE DEADLINE TO 15 JANUARY. Nominations should be submitted to:

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

Correlations, Convolutions and the Validity of Electron Crystallography -Patterson Award Lecture, 2002, San Antonio, Texas

It all started rather innocently… On 1 April 1972, we moved from Albany to Buffalo, NY. It was a beautiful, sunny, warmish, early spring day and we even had a picnic on the side of the NY State Thruway. Approaching Buffalo, we noted an ominous black cloud hovering over the city. Sure enough, as we started to unload the truck, it started to rain. "At least", said my wife, "it is not snowing". As if on cue, it started to snow.

Several days later, I walked into the Electron Optics Laboratory at Roswell Park Memorial Institute. I had a brand new NIH post-doctoral fellowship and fully expected to spend the next two years studying lipid monolayers on a water surface by x-ray scattering. Dr. Parsons looked at me and said, "We need an electron diffractionist to study hydrated protein crystals in an environmental chamber. This is your assignment." Having scarcely seen an electron microscope before, thus began my career in electron diffraction. (Donald Parsons had presented a seminar in our department at the University of Maryland School of Medicine, stating how electron diffraction might be useful for solving membrane lipid structures. At the time I had considerable difficulty in crystallizing any lipid suitable for x-ray data collection on a diffractometer. When I expressed my interest in electron diffraction as a solution to my problems, my thesis advisor dissuaded me from undertaking such work as it was too difficult a field for me. Moreover he advised me not to pursue a career in research but, rather, to find a teaching position at a small college.)

What exactly is crystallography? Structural crystallography has mostly relied on the measurement of x-ray diffraction intensities from single crystals. "Solution" of a crystal structure means finding phase values to assign to diffraction amplitudes. This, effectively, creates a high-resolution lens for a hypothetical microscope to view atomic positions within the crystal unit cell. (This explanation of diffraction in terms of conjugate planes of a lens was never obvious when I studied crystallography in graduate school, since many x-ray crystallographers are not familiar with this construct. Oddly enough, I first learned about the concept of Fourier transform pairs from an electrical engineer, turned membrane biophysicist, during my first post-doctoral study at SUNY Albany. Although then encountered in the context of signal analysis of ion fluxes across membranes it is exactly the concept that immediately clarified the underlying concepts of crystal structure analysis for me.)

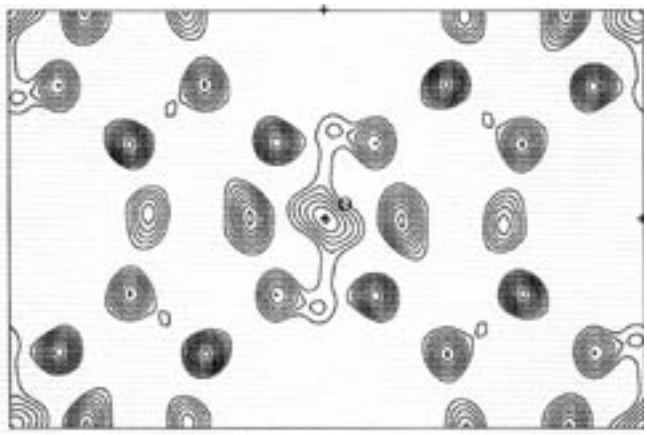
Many materials favor the microcrystalline state such that one cannot collect single crystal x-ray data and must rely instead on powder diffraction. Although there has been some progress in the direct determination of crystal structures from powder data, it is often not easy, mainly because reflection overlap presents a number of problems. These include the determination of space group symmetry, as well as unit cell constants. Separation of overlapped intensities is also not trivial, especially for high-symmetry space groups where such overlaps are exact.

In the beginning of crystallographic structure analysis, after the obvious, simple structures that could be easily solved by trial and error were examined, some other means was needed to find unknown phase terms. In 1934, A. L. Patterson saw that it was possible to apply the autocorrelation function of observed diffraction intensities (i. e. the phaseless Fourier transform of a power spectrum) for this purpose, since at atomic resolution, this is equivalent to an interatomic vector map, with all vector origins shifted to a common point. This became the primary tool for structure analysis for many years. (The correlation function and the related convolution integral figure prominently in crystallography for the description of many phenomena, including the repeat of a motif by a space lattice as well as thermal motion. An important direct methods relationship, the Sayre equation, is also expressed as a convolution. Other expressions containing these operators will be discussed below.) Later, Hauptman and Karle (and others) developed the well-known 'direct methods' in crystallography, revolutionizing the art of structure determination. Typically, crystallographic phases are expressed as linear sums, the value of which can be predicted with a probability dependent on the magnitudes of the normalized diffraction amplitudes. It is argued that, since there are more simultaneous equations than unknowns, the phase problem can be solved. A relationship between one type of phase invariant sum and the Patterson function had also been derived by Hauptman and Karle. In their paper it was stated: "It is apparent to the nature of the formulas described here that the accuracy with which phases may be determined depends on the *quality* of the Patterson function". The prophetic significance of this statement to electron crystallography will be explained below.

What is electron crystallography? If one is faced with microcrystalline materials, it is logical that a radiation more strongly scattered by matter than x-rays might be useful, particularly if single crystal patterns could then be obtained from individual microcrystals. Electrons, which are scattered 10^6 more efficiently by matter than are x-rays, fit this requirement. While the advantages for measurement of unit cell constants and determination of space group symmetry are obvious, one can also ask if the intensity data could also be used in a structure determination, in the same fashion that x-rays are. If this were possible, then we would have *electron crystallography*. For example, comparing a selected area electron diffraction pattern from a zeolite to its one-dimensional powder x-ray pattern, it is clear that there is much more information inherently in the former single crystal pattern.

The attractions of electron crystallography are several. We have already mentioned the avoidance of reflection overlap problems experienced with powder data. The small electron wavelength (100 kV electrons have a wavelength about $1/40^{th}$ that of a Cu Kα x-ray) permits collection of a complete diffraction zonal pattern at a single crystal setting since the Ewald sphere has a very large radius. As mentioned also, the strong scattering cross-section allows use of individual microcrystals for data collection. Different ratios of scattering factors sometimes means that light atoms are more visible in the presence of heavier ones than they are in x-ray crystallography. Atomic charge strongly affects the

electron scattering at low angles, theoretically facilitating the direct study of charge density distributions.



The zeolite zsm5 in projection

Indeed electron crystallography had been vigorously pursued in Moscow, beginning in the 1940's, mostly in the laboratory of Prof. Z. G. Pinsker. Instead of using an electron microscope to obtain the electron diffraction pattern from a microarea, an electron diffraction camera illuminating ~ 1-mm diameters was used instead to observe so-called 'oblique texture' patterns. While suffering from some of the overlap problems encountered in powder x-ray diffraction, the advantage of sampling such a large area was claimed to minimize the inevitable dynamical scattering interactions caused by the strong beam interaction with the sample and the excitation of more than one diffracted peak at a single crystal setting. It was claimed that only a primary (two-beam) extinction correction should be invoked when needed for such data sets.

From this arose a controversy with electron diffractionists in the West who largely depended on electron microscopes for their experiments, emphasizing single crystal diffraction and the resultant multiple beam interactions. Multiple beam dynamical scattering theory is quite complicated. For example in a series approximation, the measured dynamical structure factor amplitude can be shown to include the desired kinematical term but this is modified by higher terms including weighted n-fold convolutions of all the diffracted beams in the diffraction pattern. (For defect containing crystals, a similar series can be written to include self-convolutions of all excited zonal intensities, to be added to the desired kinematical intensity.) It was not obvious, therefore, how useful intensities could be obtained in an electron diffraction experiment for structure analysis, since the unknown crystal structure was needed *a priori* to calculate the multiple beam interactions. Although the influence of higher-order terms in the dynamical scattering model could be reduced by decrease of the electron wavelength (by increasing the electron accelerating voltage) and minimization of the crystal thickness, it was assumed without proof that the single scattering or kinematical limit must be satisfied to permit an *ab initio* structure analysis to be undertaken. An exception might be the case of thin crystals of light atom materials, for which the dynamical interactions would not be very strong.

The disagreement between electron diffractionists in the East and West was exacerbated by the Cold War. While Western researchers remained skeptical about the possibility of an electron crystallography, Russian researchers continued to report a number of structures determined from electron diffraction intensities. It was claimed, e. g. in the work of B. K. Vainshtein. that hydrogen positions in organic structures (e. g. diketopiperazine and paraffins) could be determined more accurately by electron diffraction than by x-ray crystallography. On the other hand, it was not clear how useful electron diffraction intensities would be for the determination of *new* crystal structures since many of the compounds examined in Moscow had been characterized earlier by x-ray crystallography.

(Many of these events took place in the 1950's – e. g. the latter part of A. L. Patterson's career, the development of direct methods, the formulation of the multiple beam dynamical theory for electrons, the 'electronographic' determination of crystal structures in Moscow – not to mention the deaths of Stalin and Prokofiev on the same day. I was, however, blissfully unaware of most of this as I attended Strayer's school, a model for Harbaugh's poem, "Das alt Schulhaus an der Krick" (in the Pennsylfawnisch dialect), that housed 6 grades in one room. It was equipped with outside privies and a hand-pump for water. Coal for fueling the corner stove was in the basement. I continued to be unaware of most of this all through high school and then my four years with the Brethren, although I did receive a healthy dose of German pietism with my training in chemistry.

Eventually I moved to a metropolitan area for graduate school where I was seduced by used book stores, beginning an addiction, bibliomania, that plagues me to this day. As mentioned above, we then moved to upstate New York, eventually Buffalo. My post-doctoral experience with electron diffraction at least produced nice patterns from a fully-hydrated protein and the data seemed to be suitable for structure analysis, although I had no clue how I would realize that. During that time, I attended a workshop on direct methods at the neighboring Medical Foundation of Buffalo and later was offered a job there. That lasted for 27 years via a number of grants from the NIH and NSF. We continued to practice snow-shoveling and became enthusiastic cross-country skiers, as the number of books inside increased to match the copious snowfall outside.)

The proximity of electron diffraction investigations of phospholipid structures to continued development of new direct methods by Herb Hauptman's group at the Medical Foundation of Buffalo led to the inevitable attempt to use these methods to solve a crystal structure with electron diffraction data. Indeed, attempts with data sets from two different polymethylene chain packing arrays were quite successful. However, it was thought that, since there was only one dominant scattering species, the success was probably coincidental. Later, in a collaboration with B. K. Jap and R. M. Glaeser at UC Berkeley, where test dynamical diffraction data were generated for two other more complicated organic molecules, it was found that there was a domain of crystal thickness/electron wavelength where the diffraction intensities were of sufficient quality for *ab initio* structure determinations by the tangent formula. More importantly, the criteria needed for collection of useful electron diffraction

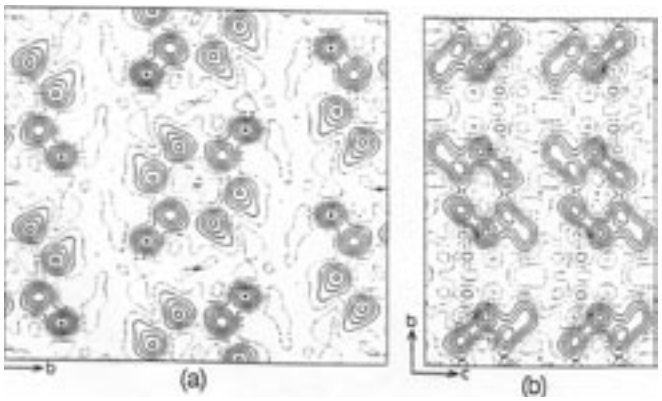
intensity data could be realized in the laboratory. This opened up the field of organic structure determination, as is described in my monograph *Structural Electron Crystallography*, published by Plenum in 1995. Application areas have included: linear polymers, polydisperse linear chain arrays, aromatics, non-linear optical materials, small molecules, and buckminsterfullerenes, very often by direct methods. Meanwhile Unwin and Henderson had published an important description of a method for protein structure determination in the electron microscope by low dose techniques, using the Fourier transform of noisy micrographs to provide phase terms for electron diffraction amplitudes. (Eventually, I was fortunate enough to spend a year's sabbatical at the University of Basel to gain some first-hand experience with this methodology in the collaborative structure determination of a transmembrane porin.)

A number of direct methods had been found to be useful in electron crystallography, e. g. symbolic addition, the tangent formula, the Sayre equation, the minimal principle, and maximum entropy and likelihood (the latter by Chris Gilmore in Glasgow, a good friend and collaborator). The reason for this success seemed to be that, even with demonstrable dynamical scattering, the clustering of large $|E_h|$ terms seemed to correspond more or less to the kinematically strong terms. Both three- and four-phase invariants were useful, and, some errors were permitted in the phase determination.

Materials containing heavier atoms were approached much more timidly, however, due to perceived problems with dynamical scattering. In 1979, Prof. Natsu Uyeda published enticing 2.0 Å electron micrographs of an organometallic dyestuff, copper perchlorophthalocyanine, at 500 kV. In these images the positions of copper and peripheral halogens could be correctly determined but the organic moiety was not at all clearly resolved. The challenge, therefore, was to complete the structure from electron diffraction data. Obtaining a suitable data set at 1200 kV at the high voltage electron microscope in Albany, NY, we found that the desired structure determination could be carried out in several ways. First, one could use symbolic addition, followed by Fourier refinement, or one could elect to extend 2.0 or 2.4 Å phases from the direct Fourier transform of electron micrographs (one of these taken by John Fryer, another good friend and collaborator) by the Sayre equation. The positions of all carbon and nitrogen atoms were found. On average all bond distances and angles were reasonable. A cosmetically similar result was found for the isostructural perbromo- analog, except that the final C-Br bonds were too short, an expected outcome of dynamical scattering.

Despite dynamical diffraction, however, the structures could be found from the electron diffraction data by direct methods. The reason for this was that the experimental Patterson function, calculated from observed intensities, continued to resemble the autocorrelation function of the actual crystal structure. In other words, the success of structure determination with electron diffraction intensities seem to depend on the quality of the experimental Patterson function, echoing the comment cited above from Hauptman and Karle, but with 'quality' meant in another way. This criterion had been anticipated by Prof. J. M. Cowley, one of the developers of the multiple beam dynamical theory, in his early attempts to solve crystal structures from electron diffraction intensities. He had exploited a power series in intensity to construct a modified Patterson function wherein details of interatomic vectors could be more easily discerned from dynamical data.

Meanwhile there was the matter of the earlier Russian electron diffraction analyses. Were these on the level? Prof. B. K. Vainshtein had been awarded the Ewald Prize by the IUCr in 1990 at the Bordeaux Congress. This motivated me to re-examine his data set from diketopiperazine. To my great astonishment, direct methods (first: symbolic addition, later: the tangent formula) solved the structure easily. Many other texture data sets from organics and inorganics obtained by the Russian laboratories could also be used for direct determinations. In other words, the Russian electron crystallographers had been correct all along but unfortunately they had not demonstrated the ability to solve structures directly from their observed data in order to quiet criticism from the West.

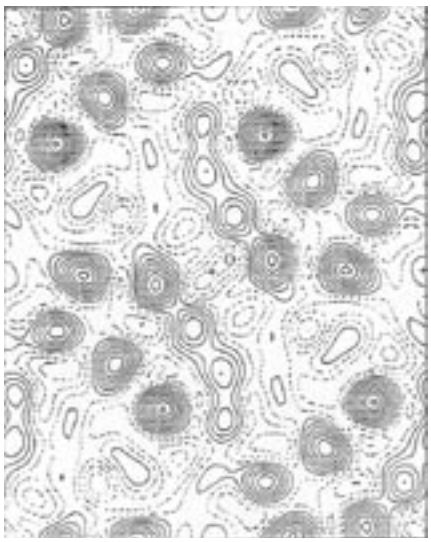


Diketopiperazine from Vainshtein's texture diffraction data

The utility of texture electron diffraction intensity data for *ab initio* structure analysis does not invalidate the existence and importance of multiple beam dynamical scattering. Two things were made clear, however, from the successful analysis of such data. First, it is advantageous to average over various crystal orientations to record true integrated intensities. Selected area electron diffraction intensities do not comprise optimal data sets. This observation led to the development of a precession mode for collecting data in the electron microscope by Roger Vincent and Paul Midgley at the University of Bristol. This method exploits the Russian result while preserving a single crystal orientation. An example of a three-dimensional structure solved from such data is that of the alloy Al_mFe by Jon Gjønnes and his co-workers in Oslo. (Chris Gilmore and I found these data to be favorable for direct methods determinations.) The second important point is that the structure analysis may be useful enough to construct a trial model, even if the R-factor agreement to the observed data is poor. (From the standpoint of an assumed kinematical model, this is a dangerous statement because one cannot demonstrate the success of a model from observed data alone without making a dynamical correction.) Numerous analyses of inorganic structures are currently reported where this is the case. Our more recent

experience is in the area of zeolite crystallography where so-called T-site positions can be found by direct methods on electron diffraction intensities. Such determinations may not be easy and secondary scattering perturbations can be problematic.

Another intriguing influence of the Patterson function on electron diffraction determinations was evidenced in the study of low-resolution data from several thin protein crystals. As David Harker originally pointed out (also in a chance discussion when he was an emeritus professor at HWI), a protein can be assumed to be an assembly of globs. If the scattering factor of a glob were known then low-resolution data scaled by its transform would lead to a more accurate data normalization than if the aggregate of atomic scattering factors were employed for this purpose. Examples include the 6 Å data sets from bacteriorhodopsin or other similar proteins. If the cross-section of projected α–helices is assumed to be Gaussian, then its Fourier transform would also be Gaussian. Since fibrous α–helical proteins place center-to-center distances at 15 Å, this suggests a 10-fold re-scaling of the data set to simulate a small molecule problem, where the glob scattering factor could be modeled accurately enough by, say, a carbon scattering factor. For centrosymmetric projections, the analysis is easy and highly accurate. For non-centric projections where symbolic terms are required, one of the structure solutions is quite accurate – it is just difficult to discern which is the preferred one since no suggested figure of merit is sufficiently robust to identify the best solution. This also underscores the ultimate need for chemical constraints for determining structures at atomic resolution but no such constraints exist for the aggregate of globs. (For the data set from hydrated catalase, the analysis was carried out easily from the electron diffraction data in plane group *pgg*, allowing me to finish my post-doctoral project 25 years late.)



Orthorhombic bacteriorhodopsin (6 Å resolution)

What can we conclude from all this? Work continues in electron crystallography in application areas not perceived just a few years ago to be possible. Obviously qualitative electron diffraction is a good technique to resolve dimensional and symmetry ambiguities left after powder x-ray experiments. This fact has never been disputed. Quantitative electron diffraction structure analysis is also quite possible for organic and inorganic materials, if proper care is made with specimen preparation and diffraction measurements.

The chief criterion for solving a crystal structure from electron diffraction intensity data is that the experimental Patterson function should adequately correspond to the crystal autocorrelation function. This constraint is quite different than the near approach to the kinematical limit, a constraint that was once assumed without proof. *Ab initio* structure analyses are possible with electron diffraction intensities and, contrary to popular belief, new crystal structures have been solved from electron diffraction intensities alone. It is therefore pleasant that this work should be associated with A. L. Patterson's career since it is the interpretability of his autocorrelation function that makes electron crystallography possible.

The main role of electron crystallography seems to be the investigation of microcrystalline materials as an assortment of individual, single crystals. There are numerous problems that are appropriate. For highly accurate structure determinations, electron crystallography will never supplant x-ray crystallography, if only because there are fewer data available in comparable optimal cases. The major challenge to electron crystallography, currently, is that of structure refinement. With electron diffraction data, constraints are required if a kinematical model is assumed. Efforts are underway, e. g. by H. Zandbergen and J. Jansen in Delft, to include dynamical calculations permitting a search for a global minimum in refinement space. Alternatively, Rietveld refinements are possible against powder x-ray data after the initial model is derived by electron crystallography.

Finally, I never was able to determine a phospholipid structure in three-dimensions by electron crystallography. This was what motivated me to use electrons in the first place but I cannot claim success.

I am very grateful to the American Crystallographic Association for the Patterson Award and for the support of those who made it possible. I would also like to thank a number of people for their profound influence on my career but cannot list them all here. I should really congratulate my thesis advisor for making me angry enough to follow my own path. It was very clever of him. I thank Harvey Fishman for being a *mensch*, igniting a passion for research, and introducing me to the concept of Fourier transform pairs. I thank Donald Parsons for making a crucial decision for me in April 1972. I thank Herb Hauptman for his support and many fruitful discussions, also about classical music, and the staff at MFB/HWI for providing a basement with an electron microscope for this work. There are a number of good collaborators and co-workers who have paved the way to successful structures and I am grateful; colleagues in Scotland, the Alsace, Switzerland and Germany have been particularly generous. I thank my wife Bonnie for bravely putting up with the vagaries of a free-lancer life with a salary totally dependent on research grants, particularly the attendant neuroses when times were tough. I also thank my son Erik for having the guts to do something similar as a musician, now as a violinist in Akademie für Alte Musik, Berlin. Finally I thank the management of ExxonMobil Research and Engineering Co. for their continued encouragement of my latest work.

Doug Dorset

ACA San Antonio Travel Awards

Thanks to the generosity of ACA members who contributed to the Etter Travel Award Fund and to our corporate supporters it was once again possible to provide financial assistance for young scientists to attend the San Antonio ACA meeting. Just under 29,000 dollars was shared by 56 awardees, 18 of whom were from countries outside the US. A full list of awardees and corporate donors was published in the Summer Newsletter (page 36). Followingare reports received from a number of the awardees detailing their experiences in San Antonio.

I definitely enjoyed the meeting and it was very informative. As a graduate student in biophysics crystallography, I was glad to get a protein structure solved months before, but I still had lots of questions about the development and future in this area. The meeting helped me to see what other people are doing and how they are thinking. I met, listened to and talked with many famous figures in this area. Previously I could only read their books, run their programs, but not talk with them face to face. I know them now. I was very intersted in the rapid development of high-throughput crystallography, and excited about the possiblities in structural genomics. I felt a pressure that I would be far behind if I had not been at the meeting. I liked the Enzyme Mechanism session, too, and was proud that there were five presentations about beta-lactamases.

To my pleasant surprise, many people came to see my poster. Some people were helpful and provided valuable comments. I have gained confidence from their friendly support. Of course, I learned more from other people's posters. I felt that I could do much better next time.

Not only did I enjoy the academic events, but also some extracurricular activities. I liked to walk along the Riverwalk, or sit down dining beside the water. The view was stylish. At the ACA dinner and mixer, some professors were very hospitable to chat with us, joking and laughing. I felt close. It is a society I am truly in. Another interesting experience was my visit to La Villita, where I met an artist. He liked to paint oriental subjects. I was happy to see his paintings. Now, I often visit his gallery web site. This meeting was an enriching experience. I am grateful to the ACA travel grant for it.

Sun Tao

First at all I want to thank the meeting organizers for the travel grant that allowed me to attend this important international event. For me all was chatty, because it was my first participation in an important international meeting. The lectures of the professors Desiraju, Gavezzoti, Aakeröy and Keller were very important for me in the development of my PhD. The poster sessions were also very useful because they allowed me to see the different work of other PhD students. I am thankful to all organizers of the ACA meeting.

Sauli Santos, Jr.

I appreciate the financial support to attend the ACA 2002 Meeting. I liked the meeting a lot.

Among other things, I enjoyed the discussion about the importance of hydrogen bonds in supramolecular chemistry and crystal engineering. I also liked a lot the discussion about detectors and data processing – data accuracy and precision are very important to good experimental work. The evening session about authorship issues was also very nice, and presented interesting features of ethics and crystallography (e.g. how structure determination should be considered in a scientific work?).

Finally, I would like to say that it was very good to see many Latin American crystallographers at this meeting. I hope it will happen again at future ACA meetings

Bernardo Lages Rodrigues

First of all I want to express my gratitude to organizers of the ACA 2002 meeting, for giving me the opportunity to attend this important scientific meeting and present my work to the international audience. It would have been impossible without the support I received.

The meeting was well organized and

took place in an atmosphere of scientific collaboration and intensive idea exchange. The interaction with other scientists presenting works in the same field as mine, as well as with adjacent fields gave me many new innovative ideas and allowed me to reinterpret and to re-analyze certain issues connected with my scientific work.

I had a wonderful time in San Antonio, visiting many interesting historical and cultural places. I was impressed by the downtown area of San Antonio, visited the Alamo museum, and learned several historical facts about Texas and San Antonio. In particular. I enjoyed the food, culture, music and hospitality.

Once again I would like to thank everybody who made it possible for me and my son Hayik (also pictured) to attend this scientific gathering in this beautiful city.

Siranush E. Bezirganyan

The 2002 ACA meeting in San Antonio this past spring was a very useful experience, and I had quite a bit of fun as well. I would like to take this opportunity to thank the ACA for providing the financial support which allowed me to participate. The conference represented a wonderful opportunity to meet new people and learn about new (and some not so new, but nonetheless important) issues in the field.

I particularly liked the"Impact of Scattering on Nanoscale and Nanotechnology" session, due to its diverse content. The talks presented were on various unrelated topics, with the only common thing being the length-scale. I also enjoyed several talks in the "General Interest" session, as well as in "From Structures to Material Science" session. The Transactions symposium "Crystal Structure Determinations From Powder Diffraction" I should also mention as it was useful for me to some extent as well.

This meeting provided opportunity for me to present our new results on solving the structure of nanocrystalline V_2O_5 xerogel, and advertise the atomic pair distribution function technique that we used as a powerful tool for investigating structure of materials with limited structural coherence.

Moreover, this was my first oral presentation at ACA meetings, and it was fun. This past ACA meeting was very valuable for my research career, and, needless to say, I enjoyed being in San Antonio. Being in his city was more than fun - it was relaxing.

Emil Bozin

First of all, I would like to thank the ACA for providing the financial support for Young scientists from Central and South America to attend the ACA 2002 meeting. It was my first ACA meeting and my first time in the USA at all. Attending the 2002 ACA conference in San Antonio was a very exciting experience. I attended many interesting seminars. Sometimes it was very difficult to choose between sessions that were going on at the same time. The poster session allowed me to share my work and it was a good opportunity to exchange scientific information and update my knowledge of Crystallography. I now know many authors of famous papers, books, and crystallographic software related to my research line. I also enjoyed the social events. San Antonio is a great place for a meeting and to visit.

Antonio Carlos Doriguetto

I had a great experience at the ACA 2002 meeting in San Antonio. While I was there I had the opportunity to interact with crystallographers from all different areas including academics and industry. This interaction will help me make more informed decisions concerning my carreer after graduate school. Being in an academic setting makes it difficult to get a sense of what industrial science is like. I now have a better understanding because of several conversations with industrial crystallographers at the meeting.

I also found the sessions to be very helpful in my basic understanding of crystallography and I will be able to apply information from several of the presentations to my own research. I also have a better sense of the future of crystallography due to presentations on robotics and high-throughput methodology.

Dave Duda

I am very grateful for the travel award that helped fund my trip to the 2002 ACA conference in San Antonio. The conference gave me the opportunity to interact with some of the leading scientists in my field. Because I am working in the field of crystal engineering, I particularly enjoyed listening to the talks concerning the problems of interpenetration in the formation of open frameworks using a modular approach. Moreover the speakers demonstrated the possibility of using these open frameworks as functional materials. I learned much from attending the sessions as well as from talking to other chemists informally during breaks or at the social functions. I found the time to network with my colleagues in the crystallographic field invaluable. I was also glad for the chance to present my poster. At the poster session, I had the opportunity to hear others' perspectives on my research and came away with new ideas to further develop my work.

Eric Elisabeth

Attending the Annual Meetings of the American Crystallographic Association over the past several years has been a superb opportunity to interact with both other young scientists as well as those pioneers who have developed many of the crystallographic techniques widely used today. The 2002 ACA Annual Meeting in San Antonio was an outstanding congregation of both academic and industrial research groups. Through the generous partial Travel Grant provided by the ACA, I had the opportunity to participate in this stimulating meeting. I truly thank the ACA for the financial support to attend the 2002 Annual Meeting. It also allowed me to present several aspects of my dissertation research (abstract entitled "A Halide Substrate Bound in the Distal Heme Cavity of Myeloperoxidase").

An unusually pleasant dilemma at the ACA meeting was the tough decision as to which seminar to attend during the concurrent sessions. On many occasions, I distinctly recall being equally interested in two or more concurrent talks! Personally, several talks were directly applicable to my research, e.g. the presentation by Professor Ethan Merritt from Washington University on the benefits of TLS refinement over fully isotropic refinement; the talk concerning the use of helium (the "Heli Toledo") rather than nitrogen cryostats for abating radiation effects during data collection by Dr. Leif Hanson of Oak Ridge National Laboratory; and the talk by Dr. Howard Robinson (Brookhaven National Laboratory) discussing data management during synchrotron trips.

During the past several years, automation and robotics have become incorporated in many aspects of protein crystallography to facilitate the rapid determination of thousands of structures necessary for the current proteomics initiatives. Not surprising, many talks and posters at the 2002 Annual Meeting dealt with these spectacular high through-put techniques. It was amazing to see the videos and robotics in action, demonstrating procedures such as crystal mounting under cryogenic conditions, structure solution from nanoliter droplets, and optical plate scanning for signs of crystal growth. For smaller laboratories, "trickle down" of this type of technology is resulting in faster setup and analysis of crystallization trials for suitable crystal forms (often the bottleneck in structure determination).

Classical methodologies were also well-represented at the meeting. As a relatively new entrant in the field of crystallography, I thoroughly benefited from the talk by Professor Bernhard Rupp (Lawrence Livermore National Laboratory) which clearly presented many instances of phase bias along with a host of methods to detect and avoid it during model building. Equally useful was Professor Jane Richardson's (Duke University) presentation which focused on detecting and correcting errors during model building. The use of web-based tools for analyzing and improving protein models was emphasized. Such readily available resources should result in more accurate PDB depositions.

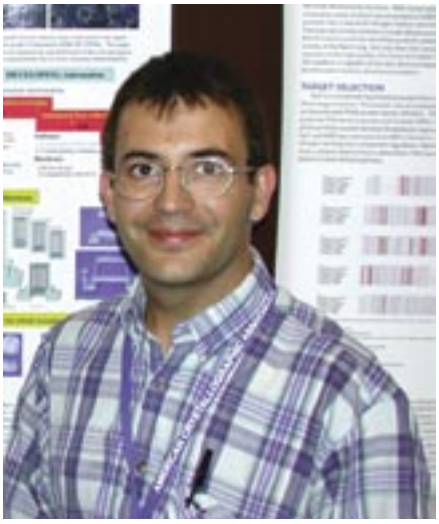
Aside from the formal seminars, the poster sessions and trade show were excellent opportunities to have discussions with colleagues and to make new acquaintances. These events were held in a relaxed yet productive atmosphere which promoted scientific discourse. I was especially interested in a poster located adjacent to mine which reported a novel structural aspect of myeloperoxidase, based on a different crystal form than I had studied during my dissertation. Similarly, the presentation on *Funding Opportunities and Effective Grant Writing for Structural Scientists* provided valuable tips on how to secure funds from public sources, a necessary component of most investigator-initiated scientific research. I must also mention the entertaining (as always!) yet informative talk by Professor Wally Cordes (University of Arkansas) on Teaching Techniques. This session was filled with examples provided by the audience of how to present many essential topics in courses on crystallography.

I again express my sincere appreciation to the ACA for the Travel Grant which helped defray much of the cost of attending the meeting. By attending the 2002 Annual Meeting, not only did I have a chance to learn about state-of-the art techniques but also to listen to leaders such as Professor Douglas Dorset (Exxon Mobil Research & Engineering), the recipient of the 2002 Patterson Award, who outlined the development of electron crystallography over the past several decades. I further conserved on finances by taking advantage of the Roommate Finder by Jeff Deschamps (Naval Research Lab, Washington DC) and staying at a nearby motel. As a result, I met another speaker, William Watson (University of Colorado Health Sciences Center) who presented his very interesting structure of Esa1, an acyl-homoserine lactone synthase involved in bacterial quorum sensing. A unexpected 'bonus' of staying at the "RiverWalk" Motel 6 was the daily

two mile walk! We should have expected this when the cab driver laughed uncontrollably as we mentioned RiverWalk and Motel 6 in the same sentence.

The 2002 San Antonio meeting of the ACA was a stimulating and motivating event. It was truly outstanding to have so much excellent structural biology presented in just a few days. Events such as the Mar Boat rides, the Young Scientists Mixer, the Rigaku/MSC Fun Run, and the Bruker/Nonius dinner added a pleasant touch to the meeting. The ACA staff also deserve special recognition for making the organizational aspects of the meeting, from registration to poster sessions, run seamlessly and on time. I am very appreciative for being able to attend the Annual Meeting and I thank the ACA again!

Tristan J. Fiedler



Wonderful place. I congratulate the advising committee for the selection of San Antonio. Thiswas my third ACA meeting; first as a student and now as a postdoctoral I have always enjoyed this reunion. From my first time in Buffalo, where the organization gave me the opportunity to present my work in a five minute talk, to San Antonio where the travel award allowed to me to enjoy again this community I have felt supported by the ACA. I would like to encourage the advising committee to continue the support of young scientists, not only through these awards but by maintaining the short presentation of selected works. I think it will be nice to see a section in which people applying to any of the three poster-prizes could present their work in a short speech.

Jose A. Gavira-Gallardo

I enjoyed the 2002 ACA Meeting in San Antonio. Although it was not my first conference I found it to be the most interesting one. My favorite session was the one on *Crystal Engineering*, which held a lot of remarkable talks and many posters. I liked *Cool Structures* as well. Surprisingly, however, I found some of them were not so cool. Overall, I liked being a part of the conference and having an opportunity to show my graduate research. During the poster session I talked to many interesting people and felt much interest in my presentation from their side. I thank the ACA for their travel grant and many thanks for awarding me the Pauling prize. It was a great and stimulating experience.

Andrey Kovalesky

I would like to thank the American Crystallographic Association for providing funding for me to attend the conference in San Antonio, Texas. This was the first conference I had the pleasure of attending, and I found the experience to be quite rewarding both academically and culturally.

I presented a poster at the conference, and the poster session allowed me to interact with both professors and crystallographers, as well as other graduate students. The feedback I received from the professors was invaluable. They not only asked questions to help me understand the material better, but also gave me tips on ways to improve my research and achieve future success. Additionally, they came up with a variety of similar but new compounds that could be easily incorporated into my research. The variety of topics presented by the professors showed how taking different approaches to problems can help one solve a whole spectrum of problems.

The other graduate students offered a very candid view of their research. They were very willing to talk not only about what had worked for them, but also about things they had tried that failed. I often found myself talking with them about reactions and techniques to avoid. This could potentially save me a great deal of time and frustration when dealing with my own research. They also gave many hints and ideas at ways to improve my current work.

Although I had not anticipated this, I also learned a great deal about other cultures while in San Antonio. Many of the graduate students attending were from foreign countries and the interaction with them both socially and professionally gave me some insight into their academic and cultural backgrounds. The many professors present also came to Texas from around the world. The variety of educational experiences helped me come up with new and exciting ideas that I would otherwise have not come up with on my own.

Brock Levin

The ACA meeting in San Antonio was my first experience at a professional gathering of crystallographers and I certainly was not disappointed. Both industry and academia were well represented and happy to answer any questions that I had. There were many great talks by world renowned speakers on all aspects of crystallography. The posters also were very informative and gave a good synopsis of many of my colleagues' research. I was also very excited to share the progress of my own research. The poster sessions afforded me a great opportunity to reach many different people. It was also very beneficial for me to discuss problems that have arisen in my own research with more experienced scientists. I am very grateful to the ACA for their generosity in extending a travel grant to me; without it, I would not have been able to attend. Hopefully, many more students will be able to attend future ACA meetings due to these grants.

Robbie Reutzel

I would like to extend my gratitude for the travel grant that helped me to attend the 2002 ACA meeting. The conference provided me a tremendous opportunity to discuss my research with experienced crystallographers at my poster session and to learn more about new developments in the field at the seminars I attended. I hope to incorporate a number of these new tools into my work. The meeting also gave me the opportunity to expand my horizons beyond my current work to other imaging methods such as electron microscopy and different techniques such as time-resolved crystallography. Not only did I gain research-related knowledge I also got my first introduction to the financial concerns I will face later in my career at the Funding Opportunities Workshop. As a graduate student, this allowed me to begin to understand how funding decisions are made and what a successful first-time funding application entails. Attending this meeting was an invaluable experience for my development as a structural biologist and I look forward to continuing to extend my professional training at future meetings.

Ursula Ramirez

First, my most sincere thanks go to the organizers and my adviser who together made my first ACA meeting possible. This participation has been quite an enjoyable and exiting experience.

San Antonio surprised me a lot by its unique characteristics, standing out from many other cities which seem to grow more alike. People there were warm and welcoming, so is the climate. It was so much fun and relaxing strolling around the River Walk after trying hard to understand meeting talks.

What impressed me most during the ACA 2002 Annual Meeting was the diversity and superior quality of talks. It's very beneficial to me, a Ph.D. student, to learn about exciting research going on in other branches of science. This meeting offered an excellent opportunity to sit back and hear what's happening around this community. Many speakers talked about their most recent progress in the lab, which brought the audience to the forefront in that area. I have to admit that there wasn't much I really understood. However, a scientific meeting is intended to bring together people of same and different interests, to let them show and discuss their work. I think the purpose of this meeting was well served.

Other elements in the meeting such as the fun run to Alamo-dome, Young scientist mixer are really great to take part in. Thanks again to the organizers for their significant amout of effort and hard work. I am looking forward to the ACA 2003 meeting.

Xiangyun Qiu

I had intended to come to San Antonio primarily to present my work and to connect with possible post-doc employers. However, the meeting proved more helpful than I had expected in other areas. I was pleasantly surprised by how many talks and posters caught my interest. By learning about other areas of research and newer technologies, I have been able to re-approach some of the challenges and questions in my own research with fresh perspective and new ideas. Many concepts were fascinating , despite being not straightforwardly applicable to my work. The discussions of new technologies were most interesting. During the session on

biomolecular crystal growth, I decided to forgive my crystals for not being perfect, so long as they keep diffracting. In any case, I will carry what I have learned into my next position and set of problems. In addition to the opportunity to meet and learn from distinguished scientists, interacting with other young scientists was highly rewarding. I was especially impressed at the level of work being done by some of the graduate students. I would like to thank the organizers for a well-run, informative and enjoyable conference, and the people at MAR for the boat ride.

Michael Godsey

As was the ACA meeting in Los Angeles last year, which was been my first one, the meeting in San Antonio was very inspiring and a great experience. As for the meeting in Los Angeles, I received an ACA travel grant that helped me to attend. And finally, as last year, I am a bit late writing this report about the meeting.

I am glad that I was able to listen to lots of interesting talks and to see many fantastic posters in San Antonio, as well as seeing the latest developments in the vendors exhibition. In addition I had the opportunity to present my own work about the identification of metal atoms in protein structures. Furthermore, I met many nice and inspiring people, some of which I already knew from other occasions, and had several interesting discussions.

I should like to thank everyone involved for a great meeting in San Antonio.

Peter Meuller

The First Jeffrey Awards.

Four Jeffrey Awards were presented at the Geneva IUCr Congress. These awards are made to outstanding graduate students in order to assist them in presenting their work at the Congress. The first Awards were each for $520, sufficient to cover registration and student housing costs. The Award Committee (Helen Berman, Martin Caffrey and Bryan Craven) was unanimous in choosing the Awardees from a total of fifteen applicants. The Awardees in 2002 were:

Daniel Riley (University of Newcastle, New South Wales) for rapid (0.9s) neutron diffraction data collection and differential thermal analysis which he used to follow a phase transition in titanium silicon carbide.

Mr Rudresh (Indian Institute of Science, Bangalore) for his de novo design and subsequent structure determination of a hairpin eicosapeptide containing 3_{10} helices with opposite handedness.

Liliana Sampaleanu (Hospital for Sick Children, Toronto) for her structure determination of duck delta1 and delta2 crystallin leading to a better understanding of the enzymatic mechanism of argininosuccinate lyase.

Martin de Yonge, (University of Melbourne, Victoria) for his precision measurements of the X-ray mass attenuation coefficient for molybdenum using synchrotron radiation.

These awards were made from a fund established in memory of Prof George A. Jeffrey. Contributions came from many of his colleagues and former students and from his family. The Jeffrey Fund is administered by the Pittsburgh Diffraction Society The next Jeffrey Awards will be in time for the Florence IUCr Congress.

Bryan Craven

Statement required by 39 U.S.C. 3685 showing the Ownership, Management and Circulation of ACA Newsletter, published four times per year for October 1, 2002. Publication No. 1958-9945. Annual subscription price is $1.75.

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2002 IUCr Travel Awards

The United States National Committee for Crystallography (USNCCr;) and NASA sponsored travel awards for graduate students and postdoctoral fellows to attend the IUCr Congress in Geneva, Switzerland. Kathryn Ely (Burnham Institute) and Howard Einspahr (Bristol-Meyers Squibb) coordinated the travel awards program and funds for the awards were disbursed by the Treasurer of the ACA, Doug Ohlendorf (University of Minnesota). Applications were received from U.S. academic institutions representing a broad range of geographic locations, and were reviewed by a selection committee: Kathryn Ely (Chair), Howard Einspahr (USNCCr representative), William Stallings (ACA representative, Pharmacia), Ronald Stenkamp (USNCCr representative, University of Washington) and Craig Kundrot (NASA representative, Marshall Space Flight Center). Thanks are due to the following individuals for posting of the announcement of the travel awards in ACA, USNCCr, IUCr web-sites and newsletters: Jeffrey Deschamps (Naval Research Laboratory), Ronald Stenkamp, William Duax (Hauptmann-Woodward), Michael Dacombe and Brian McMahon (IUCr) and Sharon Barnett and Mandy Moalem (Kenes International Congress Organizers).

Fourteen awards were made that provided funds for meeting registration, travel, accommodation and local expenses for the young scientists. Thirteen of the awardees presented posters at the Congress and one awardee was invited to make an oral presentation. These travel awards made it possible for crystallographers in training in small molecule crystallography, macromolecular crystallography and materials science to participate in the International Congress. Congratulations to the following awardees: ***Gregory S. Allen***, Oregon Health & Sciences University; ***Thomas W. Allen***, University of Iowa; ***Henrik Birkedal***, University of California, Santa Barbara; ***Dominika Borek***, University of Texas Southwestern Medical Center at Dallas; ***Lu Deng***, University of Georgia; ***Jennifer Stine Elam***, University of Texas Health Science Center at San Antonio; ***J. Matt Farmer***, Oak Ridge National Laboratory; ***Elsa D. Garcin,*** The Scripps Research Institute; ***Katherine M. Hoffman***, Oregon Health & Sciences University; ***Bin Jiang***, Arizona State University; ***Ji Hyun Lee***, University of Illinois at Chicago; ***Huiying Li***, University of California, Los Angeles; ***Michael Lufaso***, Ohio State University; and ***Malgorzata Rowicka***, University of Texas Southwestern Medical Center at Dallas.

Kathryn Ely

I am in my fourth year of graduate school in the Department of Chemistry at Ohio State doing research under the guidance of Dr. Patrick Woodward. My research has focused on structure prediction and synthesis of solid state perovskite compounds. Attending the IUCr Congress in Geneva allowed me to meet scientists from research groups worldwide. Interactions with other scientists at the meeting may result in improving and adding desired features to my software, expanding its utilization to a wider range of the scientific community. I formed friendships and found potential collaborators, and this could add new directions to my research. Networking with scientists from many universities and government labs will also assist me in my long-term goal of finding an independent research position after completion of my PhD. The 2002 IUCr congress was very educational and I would like to thank the USNCCr and NASA for their generous support in assisting me to attend the meeting.

Michael Lufaso

Thank you very much for awarding me a travel grant to help me attend the IUCr Congress in Geneva, 2002. It was a very interesting, rewarding, and last but not least, pleasant experience. There were many enlighting lectures and I had an opportunity to meet and talk to many great scientists I had known only from their writings, such as Gerard Bricogne and Lynn Ten Eyck. It was a very fruitful conference for me. Thank you again.

Malgorzata Rowicka

This is a time when many question the future of crystallography – in particular the field of 'small-molecule' crystallography (see for example the special issue of *Zeitschrift für Kristallographie*, volume 217 issue 7-8, 2002, where 94 crystallographers give their personal view on the past, present and future of crystallography). In this respect it was a particular pleasure to participate in the XIX International Union for Crystallography Congress and General Assembly in Geneva. My impression leaving the conference was one of comfort and excitement: crystallography is doing well and the quality and impact of the science performed by the crystal-

lographic community is ever-increasing. The 10 days in Geneva clearly showed that small-molecule crystallography, where my own work is mostly concentrated, is rapidly transforming itself to meet the challenges of the future. There is a general trend towards the study of the structure of real materials, i.e. microstructure and disorder, and towards even more intricate *in situ* measurements as a function of external fields, temperature and pressure. The importance of understanding these structural properties was high-lighted by the keynote lecture of J. Jorgensen (Argonne National Laboratory) who described the influence of nanometer-sized inhomogeneities on the performance of giant magnetoresistance materials and of high temperature superconductors. These studies are made feasible by the further evolution of synchrotron and neutron instrumentation, which were both discussed at the conference together with the development of the X-ray free electron laser.

Another exciting trend is the continuing development of supramolecular chemistry and crystal engineering. The field is rapidly moving towards effective synthesis of simple architectures and better understanding of the factors involved in polymorphism. A beautiful description of the fantastic level of control over which crystal face grows the fastest, and thereby control of the morphology of the resulting crystal, and even which polymorph is obtained was given in another keynote lecture by M. Lahav (Weizman Institute).

Each of the two poster sessions lasted four days. This allowed viewing and discussing most of the pertinent posters – even though choices had to be made due to the large number (>950) and very high quality of the poster presentations.

All in all this was for me a most successful conference: lots of exciting science and many interesting discussions with colleagues from all over the world. I was fortunate enough to be allowed to present my work in an oral presentation and it was therefore particularly important for me to be able to participate. I am very grateful to the USNCCr and NASA for the financial support that let me take part in the Geneva experience.

Henrik Birkedal

I arrived in Geneva alone, the only attendee from the U of Iowa and as a post-doc with only one year of biochemistry under my belt, I had no idea what to expect. I felt a bit like E. coli out of agar.

I didn't feel alone long. The opening ceremony on the sixth was pleasant, but mingling at the reception and meeting folks from the world over; listening to the live Israeli-German musicians while munching on cheese and crackers and making a new friend out of a fellow crystallographer, however far his interests from mine; indulging, yes, in the free wine and Heineken; -- all of this combined to make me feel welcome, and, if not quite at home, at least as though visiting a good friend whose language is odd but whose company is delightful.

The student mixer on the eighth at a local disco further cemented some friendships and began others. Though not "technically" invited, I joined a small band of young postdocs and professors who (with charity) conceivably looked enough like students to be let in, despite the poor excuse of having left our invitations at l'hotel. The bouncers indeed must have been gullible -- for who showed up an hour later to dance on the top of the bar but Joel Bernstein, Congressional Chairperson and rock-and-roller? Memories of that night linger, especially when I'm pipetting and still feel the ache in the thumb I sprained that night on the dance floor of Liquid Club.

I could go on and on about the eight days of keynote speeches and microsession lectures -- goodness knows, a few of the speakers did -- and though I learned a great deal about crystallography from the talks, I will leave it to my more knowledgeable colleagues to describe them.

Having made my previous sentences sufficiently complex, I'll keep my advice simple. Come to your first Congress, and you will feel welcome. Your eyes will open, and so will your horizons. And should certain organizations assist you in getting there and back again, well, take a moment to express your gratitude. I hope, in some small part, these recollections do so. And I hope as well that they encourage other novices to join us in Florence, and to understand what a wide and vibrant community we crystallographers are.

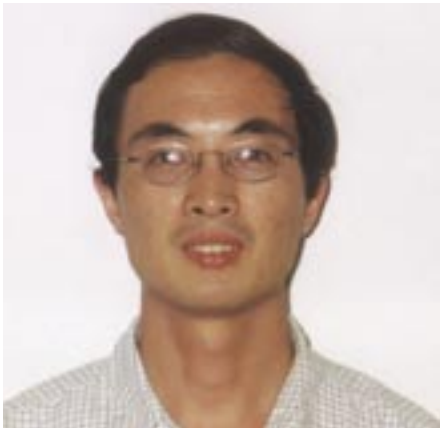
Tom Allen

I had a very enjoyable time at the conference. In addition to hearing many excellent talks, I met and got to know other students and scientists from around the world. Their company during the week was both educational and quite entertaining. The experience was particularly rewarding since my laboratory is the only crystallography lab in Portland, and while I am aware of what some other West Coast labs are studying, my understanding of the breadth of the field was somewhat narrowly focused on protein crystallography. I enjoyed the ability to take a break from protein crystallography every once in a while and pop in on a powder diffraction talk, for example. It was fascinating to see such diversity of applications. I am very grateful for the assistance provided by the USNCCr and others, which allowed for this rewarding experience.

Kate Hoffmann

As a 3rd year graduate student in macromolecular crystallography, I can't possibly overstate the positive impact of this meeting to the future of my career. I was impressed by scientific presentations that were fascinating and informative, and amazed by the broad research disciplines the meeting covered. I had to focus on lectures related to my research field, particularly hot structures, enzyme evolution and mechanism, atomic resolution protein structures, crystal growth, automation, and structural genomics. I went with hopes that I would receive and learn new ideas for my thesis project, and I was not disappointed. The people who came to my poster were pleasant, friendly and generously gave suggestions about my research problems. I was inspired in many ways by these lively discussions and came back not only with wonderful memories but also with ideas and knowledge that I was eager to try on my project. I would like to extend my sincere gratitude for your generous support.

Lu Deng



I would like to thank the USNCCr and NASA for providing funds for me to attend the IUCr Congress in Geneva. This was the first IUCr congress I have attended. It was a great opportunity for me to meet and talk to so many top scientists and broaden my view of the frontiers of crystallography. Without this support, I definitely could not have attended this wonderful congress.

At the congress, I had the opportunity to present my research on electron-diffraction, in which we map the charge density for inorganic crystals. I also had a chance to discuss with researchers who work in the field and so understand better what I am doing. It was an exciting experience to meet so many new researchers I had heard of but never met before, as well as old friends. New collaborations have also started with researchers whom I met at the conference. The congress proved both stimulating scientifically and a wonderful social gathering of old and new friends.

Bin Jiang

Attending the 2002 IUCr meeting in Geneva, Switzerland was a wonderful experience. I would like to thank the US National Committee for Crystallography and NASA for providing the travel award, which helped make my attendance possible. It was great to be able to listen to so many interesting talks and get a taste of the different research areas in crystallography around the world. In particular I enjoyed the talks in the sessions of automation of phasing, proteins of the immune system, and crystal growth of soluble and membrane macromolecules. Many poster presentations were inspiring. I wish that the poster sessions had been longer, so that I could have had more chances to talk to the presenters. Presenting my poster at the meeting was a great opportunity that allowed me to discuss my work with the scientists from different areas and gain new ideas for my research. In addition to the scientific aspects of the meeting, I also enjoyed the opportunity to meet lots of new colleagues and friends in the crystallographic community. It was an invaluable experience to attend such an interesting meeting. Besides that Geneva was a very nice place to visit.

Huiying Li

Joel Bernstein, Connie Chidister and Winnie Wong-Ng having hot chocolate on Mont Blanc during the IUCr excursion to Chaminoix on August 10th (yes - August 10th) where the temperature in the photo on the right was 23 degrees F!

Report on the XIXth General Assembly of the International Union of Crystallography, Geneva, Switzerland, 6-15 August 2002

The General Assembly was held in conjunction with the triennial IUCr Congress in Geneva, Switzerland. The scientific sessions and commercial exhibits were held in the Palexpo Exhibition and Conference Center with delegates housed in hotels throughout the city. The XIXth General Assembly and IUCr Congress were to have been held in Jerusalem, Israel, but the venue was changed to Geneva due to tensions in the mid-east. Joel Bernstein (Ben-Gurion University of the Negev, Beer-Sheva) chaired the local committee and Menahem Kaftory (Technion – Israel Institute of Technology) chaired the international program committee. The Congress drew 1,963 participants from many countries, with the largest representations from Europe, UK, Japan and the USA. Over 1700 abstracts (312 from the USA) were received, covering all aspects of crystallography and its applications. As done for the XVIIIth Congress in Glasgow in 1999, attendees were presented with a CD that contained the abstracts and other pertinent crystallographic information.

The US delegates to the Assembly were ***Marvin Hackert*** (Chair, University of Texas at Austin), ***Judith Flippen-Anderson*** (Naval Research Laboratory), ***Jon Clardy*** (Cornell University), ***Robert Sweet*** (Brookhaven National Laboratory), and ***William Stallings*** (Monsanto). The alternates present were ***Howard Einspahr*** (Bristol Myers Squibb), ***James Kaduk*** (BP/Amoco), and ***Charles Carter*** (University of North Carolina at Chapel Hill). Other alternates were ***Abe Clearfield*** and ***Ian Robinson***. All delegates were present for the first two sessions of the General Assembly. During the last session of the General Assembly, Howard Einspahr substituted for Jon Clardy who had to leave the Congress early. All delegates and alternates are either current (Hackert, Clardy, Kaduk, Einspahr, Sweet, Carter) or former (Flippen-Anderson, Stallings, Robinson, Clearfield) members of the US National Committee for Crystallography (USNCCr).

Representing the USA: (back) Bob Sweet, Jim Kaduk, and Bill Stallings. (Front) Howard Einspahr, Marv Hackert, and Judy Flippen-Anderson

The major agenda items for the USNCCr in preparation for the XIXth Assembly were the nominations for President, members of the Executive Committee, members of Commissions, venue selection for the XXIth Congress, and the proposed expulsion of Argentina. These matters were discussed at the USNCCr meeting in San Antonio, TX on May 25, 2002 and delegates were made aware of the consensus opinion of the USNCCr on matters that would be coming up for vote in Geneva. The delegates and alternates also met on two occasions in Geneva (August 7th to discuss agenda items, and August 13th to review voting procedures and strategies).

The first session of the General Assembly met on the evening of August 7th and began with an opening welcome by President Henk Schenk (The Netherlands), an introduction of the Executive Committee members, followed by a call of the roll, with 84 delegates representing 39 countries being present. The delegate from Argentina, although present, could not vote since subscriptions from their adhering body have not been paid for the past several years

No new applications for membership to the Union were originally announced, but at the last meeting it was announced that Thailand would be joining as a new Category I member. However, the matter of withdrawal of the adhering bodies from the Ukraine and Argentina were considered. Both countries have unpaid subscription dues (Category I – dues CHF 1000 or ~ $650 /yr) from their adhering bodies for several years (Ukraine since 1996; Argentina since 1998) and the Executive Committee of the IUCr, according to the By-Laws, asked the Assembly to approve the withdrawal of the Adhering bodies from the Ukraine and Argentina. Hackert from the US delegation spoke in favor of delaying such action in light of the Latin American (LA) initiatives currently underway in the United States and the prospect that a voluntary fund to assist LA crystallographers was being created. Travel assistance to meetings and schools to foster LA crystallography and improved interactions with North American crystallographers was the primary intent of the LA initiative, but it could be anticipated that the LA crystallographic community would have input as to how these funds might be used and thus assistance to help pay the subscription dues for Argentina might be possible. Delegates from Spain, Brazil, and Italy also spoke in favor of exploring ways to assist both Argentina and the Ukraine, so this matter was tabled until the next Assembly meeting on August 8th. At that meeting, it was decided to table this matter until the XXth General Assembly meeting in Florence in 2005. Thus, there are three years to sort out if this problem can be solved. Also, two countries submitted requests for changes in their Adhering Bodies. Both requests were approved. The Belgium National Committee for Crystallography reported that their adhering body is now The Royal Academies for Science and the Arts of Belgium, and the South African National Committee for Crystallography reported that their adhering body is now the National Research Foundation. There was one request for Change in Category of Adherence of Adhering Bodies, with the Adhering Body for the Czech and Slovak Republics applying for an increase from Category I (1 unit = CHF 1000) to Category II (3 units – CHF 3000).

The report of the Executive Committee of the Union was presented and accepted. Notable among their accomplishments during the past triennium was the sponsorship of numerous meetings, launching of *Acta Cryst. Section E – Structure Reports Online*, the updating of the World Directory of Crystallographers, progress with new editions of the *International Tables*, and a review of the IUCr investment policy. The Financial Report was presented by ***Sine Larson*** (General Secretary/ Treasurer) and accepted. The IUCr remains in generally good health and no dues increase was requested (the last increase was in 1993). The income of the Union is derived from subscriptions paid by the Adhering Bodies, Journal subscriptions, sale of books and *International Tables*, and its return on investments. Since 1996 the IUCr has been operating at a deficit with respect to income but the return on investments has made up the difference. However, in contrast to 1999 when an increase of 21% in fund accounts (disregarding exchange-rate fluctuations) was reported over the triennium, the past triennium saw an 18% decrease in total assets (from CHF 7,234,810 to CHF 5,934,004). However, declining interest rates and lower market returns the past few years have contributed to the decrease. The IUCr has undertaken a review of its investment policies and has adjusted its portfolio accordingly. The Union also has made a substantial investment in developing new editions of the *International Tables* and in putting Journals Online over the past three years, it is anticipated that this investment will contribute to future revenue. All journals since 1948 are now available Online.

The IUCr also maintains various funds for prizes, the Newsletter, Education, etc. The IUCr Newsletter was started in 1993. It is currently distributed to 587 libraries and over 15,000 crystallographers in 39 countries. The editor of the IUCr Newsletter has been ***Bill Duax*** from the United States and since 1999 he has also served on the IUCr Executive Committee. The Ewald Prize was presented to Professor ***Michael Woolfson*** at the meeting in Geneva. He is the sixth recipient of this prestigious award. The prize consists of a medal, a certificate and an award of $30,000. Professor Woolfson was recognized for his contributions in the development of direct methods for the more automatic solution of crystal structures (MULTAN).

The reports of the various publishing and non-publishing Commissions of the Union were presented and accepted. The Executive Committee approved a proposal to establish a new Commission on Inorganic and Mineral Structures. Reports from representatives of Regional and Scientific Associates of the IUCr (Bill Duax reported on the ACA as the regional associate) and of IUCr representatives on other scientific bodies, principally ICSU and its various committees, were also approved. A representative from each of the Committees and Commissions had met with the members of the Executive Committee before the start of the General Assembly prior to presenting their report. President Schenk reported that most of the Commissions seem to be functioning effectively in pursuit of their chartered objectives, with some comment on a lack of activity by the Commission on XAFS.

At the second meeting of the General Assembly on the 8th of August, Delegates confirmed the dates for the XXth General Assembly and IUCr Congress to be held in Florence, Italy 23-31 August, 2005. There will be seven working days (August 23-30) followed by a date for excursions on August 31st. Carlo Mealli will chair the Scientific Program Committee and Paolo Dapporto will head the Local Organizing Committee. Plans are underway for using seven parallel sessions and will include 98 microsymposia. The meeting will be held in the Congress Centre located in the very heart of the city at walking distance from the main tourist attractions and most of the hotels. The complex is made up of: *Fortezza da Basso*, *Palazzo dei Congressi* and *Palazzo degli Affari.* More information about the venue and the meeting plans can be obtained from their website at **www.iucr2005.it/** . The next item on the agenda was the preliminary consideration for the XXI General Assembly in 2008. The Delegates listened to and watched a presentation from Osaka, Japan. Japan had been proposed as a potential site for the XIXth and XXth Congresses as well. The proposed venue would be the new Osaka International Convention Center. The 21 million people near Osaka are served by the Kansai International Airport and Osaka hotels have over 30,000 rooms at various prices. The Osaka venue was the only proposal presented and was approved by the Assembly.

At the end of its second session President Schenk reminded Delegates of the Election procedures. Nominations put forward by the Exec. Committee were released by 7:30 pm Sunday. Nominations from the floor by delegates for open positions on the Exec. Committee were due by 7:30 am Monday (36 hours prior to voting) and nominations by delegates for Commissions were due by 7:30 pm Monday (24 hours prior to voting). President Schenk reported that more than 23 nominations for the 4 open positions on the Executive Committee had been received and the Exec. Committee recommended its slate of candidates based on geographical and research area considerations. Nominations from the floor require the signatures of six delegates.

At the third session the assembly of delegates voted to approve the slate of Commission members and Chairs proposed by the past chairs of commissions (based in part on the recommendations from National Committees) as reviewed and approved by the Executive Committee. The following U.S. Crystallographers were among those nominated by the IUCr Executive Committee, and elected to membership in IUCr Commissions for the 2003-2005 triennium: ***E. Arnold*** and ***M.L. Hackert*** (*Biological Macromolecules*), ***P. Montano*** and ***J. Spence*** (*Charge, Spin and Momentum Densities*), ***D. Bliss*** (*Crystal Growth and Characterization of Materials*), ***R. Grosse-Kunstleve***, ***E. Merritt*** and ***B. Vincent*** (*Crystallographic Computing*), (*Crystallographic Nomenclature*), ***J. Barnes*** (*Crystallographic Teaching*), ***J.C.H. Spence*** (*Chair*) and ***A. Eades*** (*Electron Diffraction*), ***R.J. Hemley***, ***J.B. Parise*** and ***S. Tolbert*** (*High Pressure*), ***J.D. Jorgensen*** and ***S.K. Satija*** (*Neutron Diffraction*), ***D. Balzar, C. Hubbard*** and ***R.L. Synder*** (*Powder Diffraction*), ***A. Allen*** and ***P. Thiyagarajan*** (*Small-angle Scattering*), ***Ian Robinson*** (*Chair*) and ***S.M. Gruner*** (*Synchrotron Radiation*) and ***B. Hedman*** (*XAFS*). ***J. L. Flippen-Anderson*** (*past-chair, Structural Chemistry*) will remain in a consultant capacity.

One of the IUCr's main functions is the publication of most of the leading journals in crystallography: *Acta Crystallographica, Sections A-D,* the *Journal of Applied Crystallography* and the *Journal of Synchrotron Radiation*. ***Jon Helliwell*** was reappointed as the Editor-in-Chief of *Acta Crystallographica*. ***Jenny Glusker*** (USA) was reconfirmed as the Editor of *Acta Crystallographica Section D* that concentrates on biological macromolecules and ***Carol Brock*** (USA) editor of *Acta Crystallographica Section B*. In addition, there are US Co-editors serving on all of the IUCr Journals. The Union also publishes books and a seven-volume set of International Tables covering the various areas of crystallography. Two of the seven are edited by American crystallographers: *Volume C, Mathematical, Physical and Chemical Tables*, edited by ***Ted Prince*** and *Volume F, Macromolecular Crystallography*, edited by ***Michael Rossmann*** and ***Eddie Arnold***. Finally, the Union publishes a *Newsletter* that is produced 4 times a year and sent, free of charge, to many libraries and all crystallographers listed in the *World Directory of Crystallographers*. US crystallographer ***Judith Flippen-Anderson*** was confirmed as the new Editor of the *IUCr Newsletter*, replacing ***Bill Duax*** who was nominated for President of the IUCr. Concerned with increasing costs of producing and distributing hard copy publications, as well as with the decrease in subscriptions, the Union is moving strongly towards electronic publication including CD ROM versions of journals and tables. Progress in this endeavor is good, with all journals since 1948 are now available Online.

Elections for the officers of the Union were held during the third session of the General Assembly. Several positions were unopposed in the elections. ***William Duax*** (USA) was confirmed as President of the Union, ***L.A. Aslanov*** (Russia) was confirmed as the Union Vice-President and ***Sine Larson*** (Denmark) was confirmed for a third term as General Secretary / Treasurer. ***Henk Schenk*** (Netherlands) automatically assumes the office of Past-President. The election of Bill Duax as President created a 3-year vacancy on the Executive Committee. ***Iris Torriani*** (Brazil) was nominated by the Executive Committee to fill this post; being unopposed, she was elected. The Executive Committee had presented a slate of 5 candidates for the 3 six-year vacancies for Ordinary Members of the Executive Committee (Heger / Germany; Miravitlles / Spain, Ohashi / Japan, Robinson / USA, and Vijayan / India. In addition, Judith Flippen-Anderson (USA), Judith Howard (UK), and D. Viterbo (Italy) were nominated by petition - bringing the total list of candidates to 8. The USNC/Cr had supported the nomination of Judith Flippen-Anderson and submitted her name to the Exec. Committee for consideration in 2001 and reiterated its support earlier this year. At the time the USNC/Cr met in San Antonio during late May, 2002 we did not have access to the list of candidates being put forward by the Executive Committee and voted to support the nomination of Judith Flippen-Anderson from the floor if her name did not make the slate proposed by the Exec. Committee. There was broad and enthusiastic support for her nomination, and indeed the nomination from the floor was signed by delegates from six different countries (USA, Venezuela, Brazil, Canada, Russia, and the UK). Ian Robinson's name originated from the Executive Committee. He is the 1999 ACA Warren Award winner, past member of the USNCCr, and the new chair of the Commission on Synchrotron Radiation. His nomination addressed an area under-represented on the Executive Committee. Thus there were two nominees from the USA, which may have played against either one of the USA nominees being elected. However, the process of election used by the IUCr minimizes the impact of such nominations. One must receive a majority of votes cast to be elected. ***G. Heger*** (Germany) and ***Y. Ohashi*** (Japan) were elected in the first round of balloting. If no candidate receives a majority of the ballots cast then the candidate receiving the lowest number of votes is dropped and the balloting is repeated. It took six more rounds of balloting before ***D. Viterbo*** (Italy) defeated Judith Howard and was elected to the remaining spot on the Executive Committee. Following the elections, the President adjourned the third session of General Assembly and since all business had been conducted it was not necessary to hold the scheduled fourth session.

Travel Awards to Young Scientists:

Due to the financial success of the XVIIth IUCr Congress in Seattle, the USNCCr was able to offer travel grants for attendance at both the XVIIIth and XIXth Congresses. NASA and the American Crystallographic Association (ACA) also participated in this effort. ICDD contributed to this program for the XVIIIth Congress but decided not to participate this time. Graduate students and PhD's within 3 years of graduation, citizens of or working in the USA, were eligible for the travel awards. It was also necessary to be presenting a paper (poster or oral) at the meeting. The Research and Travel Grants subcommittee of the USNC/Cr, (Co-Chairs ***Howard Einspahr*** and ***Katherine Ely*** along with ***Ron Stenkamp***) administered the program in concert with ***Craig Kundrot*** as a representative from NASA. A total of 15 awards were recommended at a stipend based on expenses up to $2000. In addition, the IUCr distributed $105,000 to support the attendance by 180 students from around the world.

Prospectus:

The IUCr is currently in good health, both scientifically and financially. The new President, ***William Duax***, is well qualified to maintain a progressive leadership role. He brings a wealth of experience to the Committee having served as President and Executive Officer of the ACA, Chair of the USNCCr, and Program Chair for the XVIIth Congress and General Assembly of the IUCr in Seattle in 1996, in additon to serving three years on the IUCr Executive Committee. Plans are well underway for the next General Assembly in Florence in 2005 (**www.iucr2005.it**/)

As with many other scientific journals the number of subscriptions to hard copy IUCr publications has been declining due to increasing costs and decreasing availability of storage space. To counteract this trend the Union has been moving strongly towards electronic publication of its journals. All journals since 1948 are now available online and new online-only versions of Journals are being introduced. The Commission on Macromolecules discussed the future possibility of a need for an *Acta Cryst. Section F* for macromolecules that could function similar to *Acta Cryst. Section E – Structure Reports Online*, but for structural genomics

and crystallization reports.

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

Marvin L. Hackert; Chair USNCCr

USNCCr Election Results (2003 – 2005)

Vice-Chair:
Jim Kaduk (BP Amoco)

Members:
Phil Bourne (USCD)
Ken Downing (LBNL)
Cheryl Klein (Xavier)
Peter Kuhn (SSRL)
John Parise (SUNY

The USNCCr is now soliciting nominations for candidates for membership to the Committee for the triennium 2004 - 2006. It is desirous to have as wide a representation as possible from the research areas that constitute crystallography and from the interdisciplinary areas that interact with crystallography. Anyone may send in a nomination. Please include the name and address of your nominee along with a short bio describing their association with crystallography.Members of the nominating committee are listed below. Send your suggestions to anyone on the committee

Joel Brock - jdb20@cornell.edu
Jim Kaduk -Kaduk@bp.com
Marilyn Olmstead - Olmstead@indigo.ucdavis.edu
Ron Stenkamp - Stenkamp@u.washington.edu

IUCr Executive Committee (2002 – 2005)

President:
W. L. Duax, USA
Vice-President:
L.A. Aslanov, Russia
General Secretary and Treasurer:
S. Larsen, Denmark
Immediate Past President:
H. Schenk, The Netherlands

Members:
M.A. Carrondo, Portugal (2005)
C. Heger, Germany (2008)
Y. Ohashi, Japan (2008)
I. Torriani, Brazil (2005)
D. Viterbo, Italy (2008)
Zhang, China (2005)

POSITIONS AVAILABLE

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

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

Faculty -X-ray crystallographer

Faculty position (open level) in the **Department of Biochemistry, University of California, Riverside,** for an individual with strong credentials in X-ray crystallography as applied to proteins or protein complexes. The specific area of research is open and can include fundamental topics such as transcription regulation, signal transduction, membrane-bound proteins, novel approaches in structural genomics, and high throughput structure determination of biological macromolecules. Available July 1, 2003. Contact: Richard J. Debus, Department of Biochemistry, UC Riverside, Riverside, CA 92521-0129; ***richard.debus@ucr.edu***

Positions Previously Listed

Postdoctoral Positions: Structural Biology

University of North Carolina at Chapel Hill: NIH-funded postdoctoral positions are available to examine the structure and action of promiscuous drug receptors (*Science* **292**: 2329), drug-processing enzymes (*Nature Structural Biology* **9**: 337), and protein-DNA complexes (*Science* **279**: 1504). Successful candidates will have experience in protein expression and purification; previous experience in protein crystallography is desired but not required. Send a CV and three letters of reference to: Matthew R. Redinbo,Depts of Chemistry and Biochemistry & Biophysics CB#3290, Chapel Hill, NC 27599-3290, ***redinbo@unc.edu***

ACA 2003 - July 26- 31
Covington, Kentucky

Abstracts Due
March 1, 2003

Advanced Registration
June 1, 2003

Advance Hotel Reservations
June 24, 2003

Update from the Proten Data Bank (PDB)

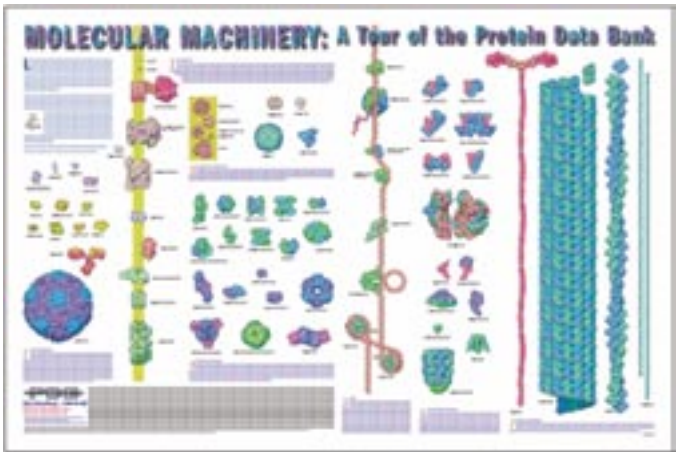
In the past year, the Protein Data Bank (PDB; www.pdb.org/) has worked on projects in a variety of specialized areas in addition to providing ongoing services such as data deposition and annotation, data query, data distribution, and outreach. A few of these projects are highlighted below.

At the end of 2002, more than 19000 structures will be available from the PDB archive. Of the structures deposited in 2002, approximately 80% percent were determined by X-ray crystallography. 91% were proteins, 4% were nucleic acids, and 5% were protein-nucleic acid complexes.

The PDB has made programs developed for data processing and annotation available (www.rcsb.org/pdb/software-list.html). These programs -- including ADIT (data editing), the PDB Validation Suite (data checking), MAXIT (data processing), and PDB_EXTRACT (extract data from structure determination applications) -- can be downloaded in source and binary versions for use on your local machines. We encourage PDB users to download these programs for use in structure depositions and to send us any feedback at sw-help@rcsb.rutgers.edu.

TargetDB (http://targetdb.pdb.org/) is a target registration database that was originally developed to provide registration and tracking information for NIH P50 structural genomics centers. TargetDB has now been expanded to include target data from worldwide structural genomics and proteomics projects. The scope of TargetDB is to provide timely status and tracking information on the progress of the production and solution of structures. Target sequences may also be searched by contributing site, protein name, project tracking identifier, date of last modification, and the current status of the target (e.g. cloned, expressed, crystallized, ...). Search results may be viewed as HTML reports, FASTA data files, or in XML.

Although many researchers are familiar with the PDB as a source of 3-D macromolecular structures and software, the repository now offers a resource that scientists, teachers, and students can pin up on a wall. .



The "Molecular Machinery: A Tour of the Protein Data Bank" poster features 75 select structures from the PDB drawn at a relative scale by David S. Goodsell. Requests for copies may be sent to info@rcsb.org

The colorful 36- by 24-inch poster is drawn at a scale of three million to one. Viewers can compare the size of a tiny water molecule to that of a giant rhinovirus or massive microtubule. It poster provides a visual tour of the molecular structures that handle various tasks in and around the cell, or "molecular machinery," as Goodsell describes it. The poster starts with a sampling of molecules that perform their duties outside the cell -- water, anitbodies, and a rhinovirus -- and progresses through the cell membrane and the various channels it contains. From there, the poster depicts transport and storage systems, enzymatic chemical factories, DNA replication, protein production, and the beams and girders that provide a cell's scaffolding.

A more detailed description of PDB activities is available in the PDB Annual Report, which is available by sending email to AnnualReport@rcsb.org.

Christine Zardecki

Update from the Cambridge Crystallographic Data Centre (CCDC)

Frank Allen took up his new position as Executive Director of the CCDC on 1 October 2002, succeeding Dr David Hartley who had been Executive Director since May 1997.

The next full release of the CSD System will be distributed on CDs from the CCDC in early December 2002. The released CSD (version 5.24) will contain 272, 066 entries. Regular CSD updates will be downloadable via www.ccdc.cam.ac.uk/ beginning in January 2003 and at two-monthly intervals thereafter. The December release also includes IsoStar Version 1.5 and new versions of ConQuest (V1.5) and Mercury (V1.1.1).

A major new feature of ConQuest 1.5 is the addition of a Hitlist Manager. This allows users to rename and annotate their searches and to generate logical combinations of hitlists. Combinations can be generated from searches, from lists of entry REFCODEs read in to ConQuest and from other combinations. It is hoped that this functionality will greatly enhance the ability of users to manipulate and organise their results. Work on improving the storage and display of data in the CSD has continued with attention being given to property data. As a result, ConQuest will more reliably display information such as crystal habit, solvent of recrystallisation and the natural source of compounds. A significant amount of work has also gone in to upgrading the ConQuest infrastructure. As a consequence performance will be much improved for searches that generate large numbers of hits.

A further new feature in ConQuest 1.5 will enable access by licensees to details of machines registered at their site and the number of licences available. The information can be accessed, using either the Help menu of ConQuest or via the CCDC's Web site, after entering the relevant Site Number and Confirmation Code. It will also be possible to purchase additional licenses on-line by credit card for immediate use.

The CCDC is also working hard on upgrading its Website, with a re-launch envisaged during the first half of 2003.

Frank Allen, Steve Salisbury, Owen Johnson & Ian Bruno

More than two-thirds of the exhibitors at the ACA meeting in San Antonio are also ACA CORPORATE MEMBERS

Advanced X-Ray Analytical Services, Inc.
www.axasinc.com

American Magnetics
www.amicanmagnetics.com

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

ATPS,Inc.
www.atpsinc.com
Bibliothek Technische Hochschule
Hanover Germany

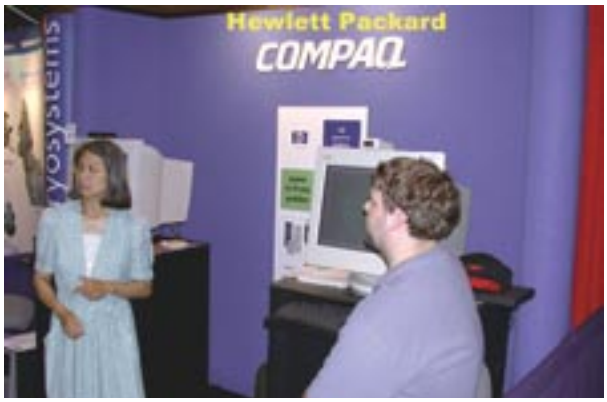
Blake Industries, Inc.
blake4xray@worldnet.att.net

Bruker/Nonius
www.bruker-axs.com

Cambridge Crystallographic Data Centre
www.ccdc.cam.ac.uk

Cartesian Technologies
www.cartesiantech.com

Charles Supper Company, Inc.
www. supper.com



Hewlett Packard
(merged with Compaq Computer Corporation)
www.hp.com

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

Crystal Logic Inc.
www.xtallogic.com

Diversified Scientific
www.dsitech.com

Douglas Instruments Limited
www.douglas.co.uk

Emerald BioStructures
www.emeraldbiostructures.com

Gilson Inc. Cyberlab
www.gilson.com

Hampton Research
www.hamptonresearch.com

International Centre for Diffraction Data
www.icdd.com

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

Microsource
www.bede.com/mirco.html

Molecular Dimensions, Inc.
www.moleculardimensions.com

MXI Systems, Inc.
www.mxisystems.com

Neuro Probe
www.neuroprobe.com

Oxford Cryosystems
www.oxfordcryosystems.com

Oxford Diffraction, Ltd.
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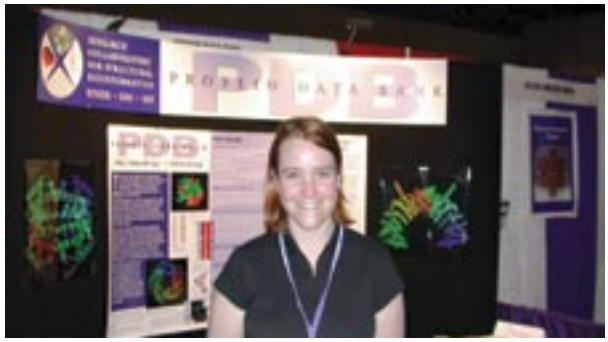

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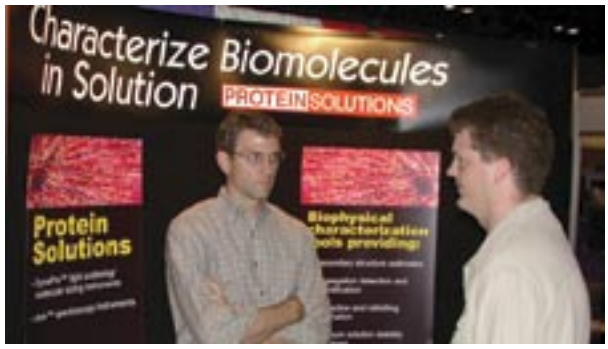

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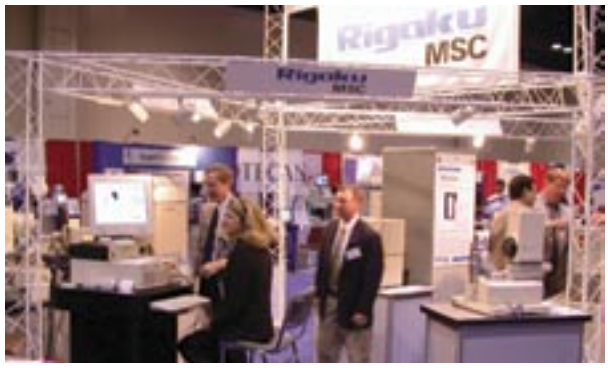

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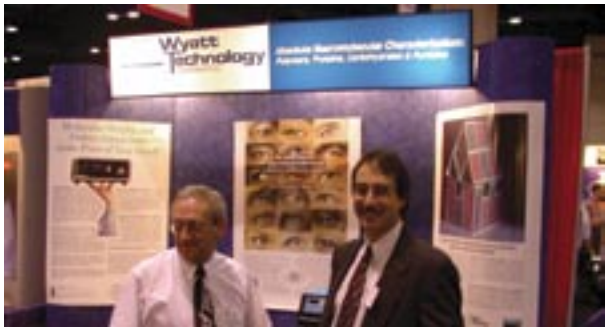

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Bob Finnegan

Doug Dorset, winner of the 2002 ACA Patterson Award. His presentation in San Antonio "Correlations, Convolutions and the Validity of Electron Crystallography" can be found on pages 14-17

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7th Annual Structural Biology Symposium, May 17-19, 2002, UTMB, Galveston

The symposium at the University of Texas Medical Branch, Galveston opened with a presentation from **Greg Petsko** (Brandeis) on indentifying the function of novel proteins using modern proteomics sleuthing methods. During a sabbatical in Ira Herzkovitz's lab, he identified a gene product YDR433 that was overexpressed in yeast cells in the G0 or quiescent phase. In addition to sequence, there are other collections of data about yeast gene products available on the web. Using these, he rapidly determined many details about this protein that a decade ago would have been stuff for several PhD theses. Shared data from microarrays showed the gene to be induced by selected stress conditions, including heat shock and peroxide, but not high salt; that it was related to 3 other genes with high sequence similarities but differing promoters; and that according to archived 2-hybrid screen data,YDR433 interacts with a group of " Snooze" gene products, also found in higher amounts in G0 phase. Finally, by using structural modeling tools, the protein was placed into a novel subfamily of cysteine proteases.

He accompanied this developing story with examples of other proteins as caution to those attempting to interpret the function of novel proteins using structural genomics. For example, the plethora of enzymes with varying activity but similar folds, such as the TIM barrels, indicates that knowing structure alone is not sufficient to predict function. Inversely, enzymes with similar functions can have quite different folds.

Moonlighting proteins

Examples throughout Greg's talk illustrated that even proteins of known activity can have other functions that may be even more relevant in their biological niches. The multifunctional, "moonlighting proteins" on his list included cytokines (endothelial cell growth factor, a.k.a. thymidine phosphorylase, and neuroleukin, phosphoglucose isomerase) and lens α-crystallins, which in addition to their structural role in the tissue of the eye, have enolase activity and sequence similarity to small heat shock proteins.

Calmodulin is a well known multifunctional protein that plays a central role in regulating intracellular response to calcium influx. **Madeline Shea** (U. Iowa) presented her group's finding that Ca^{2+} dependent changes in intrinsic fluorescence can monitor the ion binding to sites in the N-domain of the protein. While both domains are homologous, the C-domain of the protein has a 10 fold lower affinity for Ca^{2+} than the N-terminal domain in the intact molecule. Although the amino acids that chelate the calcium ions are important, interactions of distant residues provide an energetic barrier to rearranging the tertiary structure. NMR and fluorescence indicated that residues in the "flexible tether" contribute to interactions between the two domains.

They measured Ca^{2+} binding constants for a series of physiological mutants of calmodulin that interfere with its regulation of ion channels. Mutations outside the Ca^{2+} binding sites only slightly altered Ca^{2+} affinity and structural integrity, but had major effects on Ca^{2+} activated dissociation and activation of target proteins. The molecular mechanism behind these effects is now under study.

Josh Wand (U. Pennsylvania) showed how one can use novel NMR relaxation methods to estimate the contribution of the residual conformational entropy of calmodulin on binding to the target domain from the myosin light chain kinase. Methods to account for energy change on binding of protein partners rely on measurements that are either site specific (e.g., fluorescence) or global and general, such as neutron scattering or IR. NMR techniques, on the other hand, provide comprehensive site resolved information about dynamics. The complex revealed a suprising distribution of dynamics, with the amplitude of side chain motion in calmodulin segregating into three distinct classes. Analysis of other proteins indicated that these classes of motion may be a general property of proteins. Based on the distribution of side chains in each of the three classes, proteins with prosthetic groups were unusually rigid, while a designed three helix bundle protein is more dynamic than other proteins studied. Wand and coworkers have developed models to convert these dynamics into estimates of the residual entropy. Thus, calmodulin loses ~ 35 kcal in entropy upon binding its target domain. This suggests that the role of conformational entropy in dictating intermolecular interactions involving proteins can be significant.

Dynamics & entropy in autocatalytic & enzymatic cleavage of nucleic acids

Arthur Pardi (U. Colorado, Boulder) discussed another novel NMR method, to measure residual dipolar couplings of RNA molecules aligned in the presence of Pf1 filamentous phage. The phage form a liquid crystal "phage medium" in the magnetic field. About 0.1% of the nucleic acids align after colliding with the aligned phages. The Pardi group used this method to obtain long range constraints for determining the structure of the iron responsive element RNA and a valine tRNA. Further, the method revealed details of the catalytic RNA mechanisms for a lead dependent ribozyme and the hammerhead RNA. For the latter case, they found that the RNA goes through a 2 stage folding process after addition of the Mg^{2+} cofactor required for autolytic cleavage. Their local helical structures were very similar to the crystal structure of the hammerhead, which was invariant in the presence or absence of Mg^{2+}. However, their NMR studies indicated that the nucleic acid bases are more mobile and the angle between the helical stems was different in solution in the absence of Mg^{2+}. This suggests that decreased mobility of the active site residues may contribute entropically to the cleavage reaction after metal ion binding.

Linda Jen-Jacobson (U. Pittsburgh) discussed ways to estimate the contribution of release of water from nonpolar surfaces (the hydrophobic effect) to the overall energetics of specific cleavage of DNA by restriction enzymes (*Eco*RI, *Bam*HI and *Eco*RV). To measure the stoichiometric participation of water in the association of endonucleases with DNA, they measured the dependence of specific binding on the concentration and nature of small-molecule cosolutes. Their model, based on "preferential interactions" (for a completely excluded cosolute), agreed well with computations based on the surface area removed from solvent in crystal structures of restriction enzymes bound to substrate or non-specific DNA. The results imply that the hydrophobic effect provides the major driving force (up to –100 kcal/

mol) for specific-site binding. They also found that the protein and DNA surfaces remain well hydrated in nonspecific complexes, as they measure little water release and ΔC°_P values near zero.

Energetics and activity

Peter von Hippel (U. Oregon) presented an overview of transcription by the T4 phage, with emphasis on the physical and kinetic principles that enable the reaction to proceed efficiently and terminate at the proper site. Each factor in the transcription complex plays a specific role in intiating, elongating, editing, or terminating the transcript. Whether the polymerase continues or terminates the reaction at each template position is determined by the relative height of a thermodynamic barrier. Translocation is almost isoenergetic, and the polymerase reaction is highly processive. The highest energy barrier the system encounters is in the initiation steps, when the complex becomes committed to replication. Once the transcription "bubble" or opening in the DNA is formed, continued transcription is favored over termination (which may account for why termination sites often have several stop codons in a row). Premature termination can be enhanced by misincorporation, especially when the required NTP is not present at the substrate binding subsite of the polymerase, the complex is destabilized and the 3' end of the transcript can be released from the active site. Termination can be intrinsic, caused by the relative instability of the base pairing at a position, or mediated by Rho factors that compete efficiently with the elongation factor complex. This kinetically controlled view of transcription provides a useful basis for understanding how multiple polymerases, such as those that repair damaged DNA, can function on a single template molecule.

Stephen Sprang (SW Medical center Dallas) continued with another system that requires fine balancing of structural and kinetic parameters, the activation of the trimeric G-coupled proteins such as Giα, by GTP before they can bind to their appropriate cellular partner, such as adenyl cyclase. The rate of this autocatalytic reaction can be enhanced by binding of regulators of G-protein signaling (RGS). These increase the rate of GTP hydrolysis, perhaps by changing the conformation of Giα. As this sort of dynamic change would be difficult to see in the structure of RGS4 complexed with Giα, his group made alanine mutations in 3 conformationally mobile segments in Giα. They found that substrate binding and hydrolysis are uncoupled, as GTP binding is unaffected by mutants in the second helix that eliminate hydrolysis. The GTPase activating function of all RGS proteins is confined to a ~120 residue domain; however, the mechanism of all RGS molecules, such as that in p115 RhoGEF, is not identical. By using crystal structure of The RGS4:Giα complex as a model, they were able to design chimeric Gα proteins that act as substrates for p115 RhoGEF, thus revealing the source of RGS:Gα specificity.

From structure to drug design

Several of the talks addressed protein structures that could be used to design treatments for bacterial and viral infections and cancers.

James Sacchettini (Texas A&M, College Station) presented the work of a large collaboration (including the groups of Bill Jacobs (Einstein), Dave Russell (Cornell), John McKinney (Rockefeller), & Ken Duncan (GlaxoSK)) to study the structure of proteins produced by *Mycobacterium tuberculosis* and rationally design inhibitors thereof. There is an urgent need for new treatments for tuberculosis, as the existing drugs are all >30 years old and organisms resistant to them are rampant. The major problem with the current treatments is that they tend to work well against actively growing organisms but are less toxic to mycobacteria that are growing slowly within macrophages.

One possible clue to useful treatments is to observe what proteins in the pathogen are differentially expressed when an active infection becomes chronic and infectious. In active growth, the bacteria use glucose, which they metabolize through a normal TCA cycle. In the chronic phase, free glucose levels in the macrophage drop and the mycoplasma switches to beta-oxidation of fatty acids for its energy needs. During this slower, alternative metabolic phase, enzymes are induced for a variant of the TCA cycle that is not used in humans, called the glyoxylate shunt. A single enzyme converts isocitrate to glyoxylate and

Images from the 7th Annual Structural Biology Symposium in Galveston

succinate, which is converted to malate, cutting off the lower section of the cycle. While the isocitrate lyase responsible for the first step of the shunt was difficult to block, the bacterial malate synthase proved more suitable for inhibitor design. The protein has a small acidic "porthole" on its surface, that leads to a tunnel through the middle of the protein. Inhibitors designed to block this tunnel were active in the nM range and have good in vivo activity in the preliminary tests.

The structure of pathogenic viruses may also provide clues to suitable treatments. Flavivirus diseases include Dengue, Yellow fever, and West Nile, for which no treatment exists. **Robert Fox** (UTMB) showed new crystal structures of the pentameric DIII domains of Langat virus envelope protein, which are believed to interact with cellular membrane receptors. The structure provided the basis for design of small protein inhibitors, based on natural miniproteins such as tertiapin, endothelin and α-conotoxin, that could inhibit binding of flavivirus to its cellular receptor. A miniprotein that bound tightly to the DIII domain slowed the lethal effects of a flavivirus in an animal model.

Robert Davey (UTMB, Galveston) presented another model system for designing inhibitors of viral entry into mammalian cells. He presented the pathway by which murine leukemia virus (MLV, a positive strand retrovirus) enters cells. As MLV entry is protein mediated and non-pH dependent, it is a good model system for directly designing inhibitors. The envelope protein of this virus resembles closely that of human leukemia, HIV and Ebola viruses in the C-terminal region. There are 2 variable regions in the N-terminus, however. They used these sequences, produced in glycosylated form in insect cells, to clarify the interaction of the viral and cellular protein. Further analysis of an MLV isolated from a mouse infected with MLV causing limb paralysis revealed only a few mutations in the envelope protein. These mutations do not significantly reduce receptor binding but lead to higher neuroinvasiveness.

Inhibitors that block binding to members of the erbB/HER family of epidermal growth factor (EGF) receptors are being developed for cancer treatment. Herceptin, which blocks binding to the HER-2 receptor, is protective in up to 30% of breast cancers. However, several other Her-receptors may play a role in human cancers. **Dan Leahy** (HHMI, Johns Hopkins) presented a new structure for the extracellular region of another member of this family, HER-3. HER-3 has a 4 domain structure held together by 25 disulfide bonds. EGF binds HER1, which is expected to have a similar structure, at a site formed by domains 1 and 3. Elements of this binding site are ~60Å apart in the HER3 structure, indicating that a significant conformational change must occur to bind EGF, which has a longest dimension of ~30 Å. The 4th domain does not play a role in the binding to EGF, but Leahy suggests that it stabilizes the way the structure "snaps" together via an unusual interaction with domain 2. The structure gives a basis for designing two distinct types of inhibitors of binding, "snap inhibitors", cyclic peptides which could interfere with the way the receptor domains interact, or mutants of EGF that could bind but not induce conformational changes in HER-3.

And back to virtual proteomics

In the closing talk of the symposium, **Olivier Lichtarge** (Baylor College of Medicine Houston) returned to *in silico* methods of identifying the function of newly discovered proteins, by combining structure with evolutionary clues to locate active sites in proteins. He pointed out that most active site interfaces cannot be predicted from structure alone. His methodology provides a cheap, scalable alternative to site directed mutatgenesis for characterizing which residues in a novel protein control function. By combining clues from aligned sequences of great evolutionary distance and mapping conserved residues on the surface of a structure, one can identify the active site in an unknown protein by characteristic clusters of residues at the surface. His group has already applied this "evolutionary trace method" to many model systems, including mapping the DNA binding site of a nuclear receptor, the binding sites of a regulator of G-protein coupled signaling, and the distinguishing marks of rhodopsin related proteins. They identified a pattern of amino acid changes that distinguished the G-protein coupled eucaryotic rhodopsins from bacteriorhodopsin. Finally, he showed how the method could be extended to genomics by selecting 46 proteins with a variety of folds, and showing their evolutionary traces matched their active sites.

Posters

Once again, the judges had a hard time deciding on only 3 prize winners in each category among the many good posters. The 1st prize student winner was **Richard Mursinna** (University of Houston), on introducing mutants, designed rationally based on structure, into leucyl-tRNA synthetase to alter its specificity. This project also yielded a 3rd prize for **Amy Williams**, from the same group. The 2nd prize winner was **Josephine Ferreon** (UTMB) for studies on the role of conformational fluctuations on binding. Part of the shared 3rd prize went to **Ioannis Vakonakis** (Texas A&M), for work on KAIA, a circadian clock protein. The 1st prize post-doc winner was **Beatrice Huyghues-Despointes,** Texas A&M, for studies on the changes in pK values of histidines in folded and unfolded RNAse SA in differing salts. The 2nd prize winner, **Melissa McCornack**, Texas A&M, used NMR to study the GAG binding properties of the anti-HIV chemokine MIP-1B. The 3rd prize went to **Munia Mukherjee**, UTMB, for NMR characterization of miniprotein ligands.

Catherine H. Schein

8th SCSB Symposium

May 24, 2003

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MacCHESS 2002 Workshop, June 18-19, Cornell University

"High-Throughput Crystallography and Complementary Methods" was the theme for this year's meeting of the users of the macromolecular structure facility of the Cornell High-Energy Synchrotron Source (MacCHESS). The workshop brought together researchers in a broad range of fields to discuss new technologies relevant to high-throughput crystallography. As in previous years, the MacCHESS workshop was held in conjunction with the general CHESS User's meeting.

In his Tuesday address, associate director **Quan Hao**, noted several exciting new improvements to the protein crystallography beamlines at MacCHESS. The dual Quantum 4 detector system on the F1-line offers unprecedented coverage for high-resolution and large-unit-cell work. The station has also been re-tuned for SAD capability (the Br K-edge). Liquid Nitrogen plumbing for automated cold-stream maintenance is now fully operational in the F-line hutches and a similar improvement is being implemented for the A1 station. A 64-processor Linux supercomputer for fast data processing is available to users (Art Weaver's talk later in this report). Due to these and other improvements, the average time for each user visit has dropped to 40 hours, (6 hours per data set). The increasingly popular FedEx crystallography program is a new, cost-effective option for users that makes very efficient use of beamtime. There were about 140 MacCHESS related publications in the last year including a number of structures making the covers of important journals.

Brian McClain of Harvard University also spoke Tuesday on the crystallographic structure of the Rotavirus Double-Layered Particle at 5.5 Angstrom resolution (they expect to achieve 3.8 Angstrom shortly). Rotavirus is a 62,900 kDa human pathogen and a leading cause of death in the third world. In addition to conventional dual-image plates (20k spots/plate), the new dual Quantum 4 detector system at F1 station was used. Rotavirus is one of the few very large virus structures solved to date and it may provide insights into membrane enveloped viruses - a class which does not form well-ordered crystals.

Rob Thorne (Cornell) opened the morning session with a talk on his recent work about on the origin of mosaic spread in flash-cooled protein crystals. The difference in thermal contraction between amorphous ice and protein creates ice pockets within the lattice that lead to the formation of microscopic domains. Careful matching of the expansion coefficient of the cryoprotectant with that of the protein lattice could significantly reduce mosaic spread. Thorne demonstrated that microdomains caused by flash cooling can be recombined by warming the crystal to just above the water-glass transition (150K). He also described a device invented in his lab that can warm and cool the cryostream rapidly for this purpose. More details can be found in *Acta Cryst.* **D58** 459 (2002).

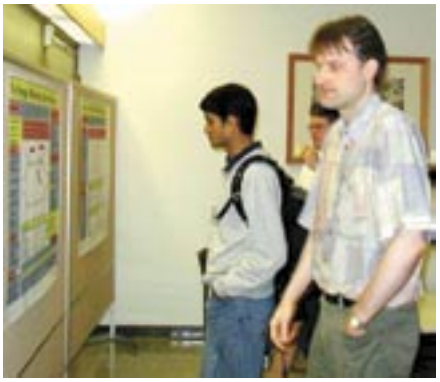
The second talk of the morning was given by **Zbigniew Dauter** (NCI & Brookhaven National Laboratory) on the use of Single-wavelength Anomalous Dispersion (SAD) for phasing protein diffraction data. Anomalous scatterers can occur naturally in a protein (sulfur, phosphorous or transition metals) or can be introduced (selenium or halides). Recent advances in both hardware and software now allow structures to be solved on a single (peak) wavelength. High multiplicity in measurements, however, is a key factor for success. Dauter recommends collecting peak data first and attempting to solve the structure on the single wavelength while the next MAD wavelength is still being collected (the so-called 1 Å wavelength method). Reprocessing of historical MAD data sets indicates that, in many cases, SAD is sufficient to solve the problem. The method is well suited for use in high-throughput environments.

Martine Cadene (The Rockefeller University) outlined the many uses of mass spectrometry in protein crystallography. When a protein fails to crystallize, it is often possible to do a partial proteolytic digestion to determine which subdomains are more structurally compact. Matrix-Assisted Laser Desorption Ionization (MALDI) is a popular and effective tool for following the progress of such digestions. Proteins of nearly 50,000 Daltons can be routinely observed. Cadene presented a special thin layer method for sample spot preparation that enhances sensitivity (see Cadene and Chait in *Anal. Chem.* **72**, 5655-8). MALDI mass spectrometry can also easily distinguish between native protein and selenomethionine derivatives.

Martine Cadene from The Rockefeller University answers questions after her talk on the uses of mass spectrometry in crystallography.

Recent innovations in the reconstruction of biomolecular structures from small-angle solution scattering were discussed by **J. Gunter Grossmann** (CLRC Daresbury Laboratory) in a joint session between the MacCHESS and CHESS workshops.

X-ray scattering profiles in the 50 to 8 Å range yield information about the overall shape of a protein. Protein scattering signals are obtained by subtracting blank buffer profiles from those obtained with protein solutions at a range of concentrations. Molecular shapes can be reconstructed using spherical harmonic expansions or bead models, the latter being capable of resolving some internal detail. Conformational changes that occur as a result of complex formation have been observed. Low-resolution molecular shapes have also been used by Grossmann and Hao to help phase diffraction data.



Gunter Grossman of Daresbury Laboratory inspects posters between sessions.

Don Bilderbach and Richard Gillilan present an award to Matt Renzi and Alper Ercan (not shown) of the Gruner group at Cornell for their poster "Pixel Array Detector for Microsecond Imaging.

Art Weaver (AJW Research) showcased the new MacCHESS supercomputer he designed in collaboration with Frank Labonte (CHESS & MacCHESS). The 31 diskless dual-processor Athlon nodes are interconnected with a Myrinet 2 Gbit/sec low latency optical switch for high-speed distributed parallel computing. The nodes run the RedHat 7.1 SMP Linux kernel. Parallel tests were performed on SnB (Shake-and-Bake phasing), MPI_FSEARCH (molecular replacement) and WebXDS. Weaver phased a selenomethionine epimerase containing 70 Se sites in 39 minutes, a task that took 17 hours on 2 processors. This single rack-mounted system, nicknamed Sirius, weighs in at more than 450 Kg (1000 lbs). The power consumption is about 8 kW, with a cooling requirement of more than 27,000 BTU/hr. Weaver warned future cluster builders to always estimate power consumption and cooling requirements, and to seriously consider low-power alternatives such as Green Destiny developed by Los Alamos National Laboratory. Complete details on Sirius, including benchmarks, can be found on the web at *staff.chess.cornell.edu/~weaver/sirius.html*.

For the first time, CHESS and MacCHESS sponsored a joint poster session competition. Three awards were given: best science, best instrumentation and best graphic design. Organizers and members of the workshop executive committee evaluated the posters during the two meeting days and presented awards on the final afternoon. Both the best science and best graphic design went to a single poster created by **Peter Bush**, **Friedrich Kremer, Christine M. Papadakis** (U. Leipzig), **Dorthe Posselt** (Roskilde U. Denmark) and **Detlef Smilgies** (CHESS) and entitled "An X-ray Reflectivity and GISAXS Study of the Lamellar orientation in Thin Biblock Copolymer films". The best instrumentation award was given for "Pixel Array Detector for Microsecond Imaging" by **Alper Ercan** and **Matt Renzi** (Gruner group, Cornell).

Phil Sorenson, Richard Gillilan, Adam Fennefrock (University of Pennsylvania) and Erie Fontes discuss new opportunities for joint software development.

This meeting was organized by Richard Gillilan, Quan Hao and director Dan Thiel. Suggested topics for future meetings may be forwarded to the organizers: *reg8@cornell.edu*. MacCHESS is supported through NIH NCRR grant RR-01646.

Richard Gillilan

ACA Dues are Due

Please pay your dues and add a little something extra for your favorite ACA fund.

60th Annual Pittsburgh Diffracton Conference, October 3-5, 2002

The 60th Annual Pittsburgh Diffraction Society Conference was held in the Holiday Inn at the University Center in Pittsburgh, PA on October 3-5, 2002. The meeting was well attended with approximately 70 attendees. The first session on Thursday afternoon, "In Memoriam: Richard McMullan", was organized and chaired by Bryan Craven. Neutron diffraction studies on a variety of compounds were presented by the many of the speakers, and the topic of two talks described X-ray crystallographic results on biological systems. All of the speakers reminded us of the huge contribution that Richard McMullan made to neutron diffraction techniques and many anecdotal stories about Richard were fondly remembered. The topic of Friday's session was "Crystallization Issues" and was organized and chaired by John Rose. In this session, many aspects of both small molecule and macromolecular crystallization were presented, including membrane proteins, high throughput, and factorial screening. Saturday morning's session, organized and chaired by Tim Umland was devoted to membrane proteins and prions. On Saturday afternoon Tim organized a session, "Protein Crystallography–Twixt Form and Function" to honor Martin Sax. In this session, talks were presented by some of Martin's former students and colleagues. All of the speakers reminded us of the role that Martin played in educating and encouraging all of those that worked around him.

The Sidhu Award was presented to Yongjae Lee of the Physics Department at Brookhaven National Laboratory. Yongjae Lee presented a very interesting talk entitled "Pressure in Nanopores" and discussed his work in the pressure-dependent chemistry in nanopores.

Fifteen posters were presented at the poster session and students were the co-author of eight. The Chung Soo Yoo Award, given to a graduate student presenting the best poster, was presented to Liliana M. Sampaleanu of The Hospital for Sick Children in Toronto, Ontario. The title of Lili's poster was "Insight into the Enzymatic Mechanism of Argininosuccinate Lyase".

In addition to two and a half days of outstanding scientific talks, all of us enjoyed renewing old acquaintances. A good time was had by all attendees at the opening reception that followed the poster session on Thursday evening. Over 60 people attended the banquet on Friday where a fine meal and liquid refreshments were served.

Dave Smith

Colorado Springs, Colorado provided the picturesque setting for the the 51st Annual Denver X-ray Conference (July 29 - August 2, 2002). Approximately 300 attendees gathered from 17 countries to discuss state-of-the-art techniques and indications for future developments in XRD, XRF, and related disciplines. In addition, over 200 exhibitors, representing 42 companies, displayed their products and communicated their services at the conference.

Organized by ***David F. Rendle***, The Forensic Science Service, Metropolitan Laboratory, London, United Kingdom and the late ***Ron Jenkins***, Emeritus, International Centre for Diffraction Data, Newtown Square, PA, this year's plenary session entitled, "Applications of X-ray Analysis to Forensic Materials", provided some rather interesting and fascinating presentations. The speakers included ***M.H. Liberman***, US Customs Laboratory, San Francisco, CA; ***D. Kloos***, Industry Consultant, Westminster, CA; ***W. Kugler***, Forensic Science Laboratory, ***Landeskriminalamt Baden-Wuerttemberg***, Stuttgart, Germany; ***D.C. Ward***, Federal Bureau of Investigation, Microanalysis Laboratory, Washington, DC; ***D.F. Rendle***, The Forensic Science Service, Metropolitan Laboratory, London, United Kingdom; and ***M.C. Bottrell,*** Federal Bureau of Investigation, Geologist/Forensic Examiner, Washington, DC.

The plenary also included a tribute to two members of the Denver X-ray Conference Organizing Committee who had recently passed away – ***Ron Jenkins***, Emeritus, International Centre for Diffraction Data, Newtown Square, PA, who passed away in June 2002, and ***Deane K. Smith***, Emeritus, The Pennsylvania State University, University Park, PA, who passed away in September 2001. The special contributions of these two pioneers will long live in the programs and structure of the conference, as well as in the history and development of X-ray analysis.

Several awards were presented at the conference. The 2002 Birks Award, recognizing outstanding contributions to the field of X-ray spectrometry, was presented to ***Michael Mantler***, Vienna University of Technology, Vienna, Austria. ***Jay C. Hanan***, California Institute of Technology, Pasadena, CA was the recipient of the 2002 Jerome B. Cohen Student Award, established to recognize exceptional achievements of student research in X-ray analysis. Honoring scientists whose distinguished work improves the Powder Diffraction File®, the 2002 McMurdie Award was presented to ***Camden R. Hubbard***, Oak Ridge National Laboratories, Oak Ridge, TN. Congratulations to all!

Yohichi Gohshi (right) presents the Birks Award to Michael Mantler (left)

Bob Snyder (left) presents the 2002 McMurdie Award to Cam Hubbard (right)

Overall, the conference included 16 tutorial workshops and 15 special sessions, in addition to the plenary. More than 100 posters were presented in three poster sessions. Topics included fundamentals of XRD and XRF, methods of phase identification, layered materials, advances in database technology, texture analysis, optics, polarized optics, Rietveld analysis, synchrotron applications, specimen preparation, quantitative analysis, TXRF, microbeam analysis, stress analysis, industrial applications of XRD & XRF, neutron diffraction, line broadening, thin films, XRF problem solving, and new developments in XRD & XRF instrumentation.

In addition to the technical programs, the attendees and exhibitors enjoyed several receptions sponsored by various vendors throughout the week. Bede Scientific, Inc., Corporation Scientifique Claisse, and SPEX CertiPrep, Inc. sponsored the Sunday evening "Welcoming Reception." Monday evening's reception was sponsored by Philips Analytical, and was held concurrently with the first XRD poster session. Materials Data, Inc. and Rigaku/MSC sponsored Tuesday evening's social, held along with the second XRD poster session, and Bruker AXS, Inc. was the sole sponsor of the Wednesday evening reception, which also included the XRF poster session.

Front: Eileen Jennings, Donna Barry: Middle: Bob Snyder, Sheila Snyder, Terry Maguire, Denise Flaherty, Jim Kaduk, Leah Mooney. Back: Cam Hubbard

Special thanks are offered to all those who participated in the conference, most notably, our session organizers, invited speakers, workshop instructors, exhibitors, and of course, our very talented Organizing Committee. The volunteer efforts of all those individuals, coupled with their enthusiastic dedication to serving the scientific community, are the key ingredients for the continuing success of the Denver X-ray Conference.

Terry Maguire

American Conference On Neutron Scattering - Inaugural Meeting: Shull Prize Announced

Directors of the U.S. neutron scattering centers, the ACNS conference chair and the NSSA president. Left to right, Jim Roberto (ORNL), Herb Mook (ORNL), Paul Lisowski (LANSCE), Rob Briber (University of Maryland), Mike Rowe (NIST), Thom Mason (SNS), Ray Teller (IPNS), Alan Hurd (LANSCE) and Jim Rhyne (Univ. of Missouri).

The Neutron Scattering Society of America (NSSA) organized the first American Conference on Neutron Scattering (ACNS) on June 23-27, 2002, held in Knoxville, TN. Attended by over 400 scientists and engineers from 13 countries, the multi-disciplinary ACNS was sponsored by the national neutron centers with assistance from the National Science Foundation and the U.S. Department of Energy (DOE). The conference, the largest on neutron science ever held in the U.S., included more than 250 papers in the fields of biology, soft condensed matter, magnetism, instrumentation, fundamental neutron physics, chemistry, and industrial applications, all with the common thread of neutrons for research. The ACNS also served as a national meeting for present and potential users of the neutron research centers at Argonne, Chalk River, Los Alamos, National Institute for Standards and Technology (NIST), and Oak Ridge, and provided an opportunity to gain insight into the capabilities and available instrumentation at these facilities. Tours of the Spallation Neutron Source (SNS) Project and the High Flux Isotope Reactor at Oak Ridge National Laboratory were also available.

Teresa Hill of Clemson University discusses her poster on solvent diffusion into ionomer thin films with Zhibin Li from the University of Tennessee.

Mike Rowe, Director of the NIST Center for Neutron Research commented: "NIST was very happy to help sponsor the first ACNS. The meeting was a great success, with many new and young attendees, who were rightly excited by the possibilities opening up with the upgrades at existing neutron sources, and the SNS construction well under way." **James Roberto**, Oak Ridge Associate Director for Physical Sciences added "We are extremely pleased with the response of the scientific community to the first ACNS. The large and enthusiastic participation foretells a promising future for the field." Locations of future ACNS meetings will rotate among the North American neutron centers with the next conference in 2004. The complete ACNS website, with the program, the invited and keynote presentations, and all of the photos, is located at http://www.sns.gov/acns.

In opening remarks, NSSA President **James Rhyne** announced the establishment of the Clifford G. Shull Prize in Neutron Science of $5,000 to be awarded every two years. Shull shared the 1994 Nobel Prize for Neutron Scattering with Canadian researcher Bertram Brockhouse. **Iran Thomas,** Deputy Associate Director of DOE Basic Energy Sciences remarked "I can not think of anything more appropriate for neutron scattering than the establishment of the Clifford G. Shull Prize. He was one of the creators of the field of neutron scattering, and it was fitting that the announcement was made close to where his work started." Thom Mason, Director of the Spallation Neutron Source (SNS), currently under construction, added "Professor Shull carried out his Nobel Prize winning research at Oak Ridge National Laboratory, and we look forward to continuing the tradition he established at the upgraded HFIR (High Flux Isotope Reactor) and soon at the SNS." **Robert Shull**, son of the Nobel prize winner and the leader of the Magnetic Materials Group at NIST presented a review of Cliff Shull's life and accomplishments to the ACNS attendees. Nominations will be solicited by the prize committee starting next year with the winner of the first Shull Prize to be announced at the 2004 ACNS.

Julie Borchers

"Polymorphism of Organic Compounds" by Joel Bernstein, Clarendon Press, Oxford, May, 2002; the latest Oxford Science Publication in the IUCr series of Monographs on Crystallography. The book has 410 pages plus 14 pages of *Contents* and Author's *Preface* and over 200 line-drawn figures and schemes. Hardcover, *ISBN* 019 850605 8. The scientific community has been presented with a long-awaited book on polymorphism. It comes from a world-renowned expert in this field, Prof. Joel Bernstein (Ben-Gurion University, Beer Sheva). His three-decade long scientific interest in polymorphs has been marked by many well known achievements such as descriptions of conformational, disappearing or concommitant polymorphs and jumping crystals, as well as development of graph descriptors for hydrogen-bonded patterns commonly used for comparisons of molecular aggregation, particularly in polymorphs.

Personally, I was already exited by the titles of sections and subsections in the *Contents*. Then I 'swallowed' all the chapters one by one in a few days. The scope and purpose of the book are outlined in the *Introduction*. Obviously he had to make choices from the thousands of substances referred to as polymorphs in literature, to which related subjects should be included and, even more importantly, which of many definitions of polymorphism to accept. His decision to take the least restrictive approach of *supramolecular isomorphism* was a good one. Although written by a chemical crystallographer mainly for chemists, crystallographers, material scientists and pharmacists, the book will also appeal to specialists in related sciences. It is written in an easy style that takes us back to the first observations of polymorphism and follows its history up to the present.

Over the last decades the subject has constantly become more of a concern to the scientific community. Any scientist involved in crystallography, materials sciences, solid-state physics, chemistry or pharmacology, must be aware of the possible polymorphic modifications of any given substance. No type of compound is exempt, polymorphs occur among small-molecules, medicinal drugs, pigments, explosives, fats, charge-transfer complexes, inclusion compounds, polymers and proteins. The different properties of polymorphs make the subject ideal for studying structure-property relationships, and essential, or even obligatory, for technological applications in chemistry-related industries. Polymorphs may differ in color, therapeutic activity, thermal or electric conductivity. Even fats in chocolate may melt and taste differently. Bernstein's book is a rich and comprehensive compilation and illustration of the structural variety of polymorphs and their properties.

There is also a chapter on legal issues related to polymorphs in industry, and litigations over the patent protection of medicinal drugs. The book can be recommended for all researchers working on organic materials, or any materials indeed. It will be of interest to academic lecturers, who will find additional illustrations for their lectures, and to undergraduates studying structural or materials sciences. The huge list of about 1500 references to scientific articles, conveniently cited with their titles, guides the reader to original and complementary sources. Page numbers added to references, direct one back to where they are cited. The *Index* (10 pages), also facilitates reading and quick location of a subject of interest. Today's instrumentation and powerful computers make it possible to rapidly perform structural analyses at various temperatures and even to do charge density studies of proteins. Powder diffraction experiments resolve two or more phases of increasingly complex substances, while theoretical predictions of the crystal structures become more efficient. With these facilities at hand, appropriate education and awareness of the polymorphism is crucial. Today's knowledge of the field of polymorphism appears as the top of an iceberg, and Bernstein decleares that one purpose of his book is to be a platform for future research. 'Be wary of the *polymorph*, that slyly lies in wait' in your laboratory, and its scientific and economic implications!

Reviewed by Andrzej Katrusiak,

"Frozen Light: The Crystal Poems" by Harvena Richter. The Wildflower Press, P.O. Box 4757, Albuquerque, New Mexico 87196-4757 (2002). This is a collection of short freeform poems about crystals, all of which I found charming and refreshing. The Albuquerque address of the author and one statement in the Foreword referring to lore about the "healing properties" of crystals made me so apprehensive that I almost did not read the book, but I felt rewarded by persisting because they do not in any way offend my scientific sensibilities with "new age" rhetoric. Rather, they convey the author's sincere appreciation for crystals in 26 different vignettes. The following is number seven:

Geode

A roundish rock
light and hollow;
you crack it open
like a nut
and find inside
a sight to startle:
pinnacles and towers
of bristling crystal,
amethyst, jasper,
chalcedony, quartz-
a hidden city
rayed with light,
a purse laden
with lustrous coin,
the inner kingdom
the heart searches.

Harvena Richter's poetry has appeared in *The New Yorker* and *The Atlantic* and she has published a novel, *The Human Shore*, and several non-fiction books including *Writing to Survive: The Private Notebooks of Conrad Richter* (her father).

Reviewed by Connie Chidester

"IUCr Teaching Pamphlet No. 2 An introduction to the scope, potential and applications of X-ray analysis" by M. Laing. has been translated into Spanish by O. C. Alonso, F. S. de Jesús, J. C. Alonso and A. M. B. Miró.

"IUCr *Teaching Pamphlet No. 20 Crystals - A Handbook for School Teachers*" by Elizabeth Wood has been translated into Arabic by Karimat El-Sayed and Boshra Awid.

"A Matter of Degrees: What Temperature Reveals About the Past and Future of Our Species, Planet, and Universe", by Gino Segrè. Illustrated. New York: Viking (2002). Of the three fundamental methods of measurement-time, length, and temperature-Gino Segrè is convinced that temperature is not only the most subtle but also the most revealing. In this engaging, insightful book, Segrè, a distinguished theoretical physicist, makes his lifelong fascination with temperature the organizing theme of a wide-ranging journey through science, history, and culture. A graceful writer and a nimble synthesizer, Segrè explores how temperature (which we have only recently succeeded in measuring) is bound up with the very essence of both life and inert matter. Why is the internal temperature of most mammals fixed at 98.6 degrees, no matter what climate they inhabit? What do the hydrothermal vents on the ocean floor reveal about the history of our planet? Why has temperature proved to be so much more difficult to measure than distance and time? How does the quest to reach absolute zero relate to the problem of superconductivity in quantum physics? In answering these and hundreds of other temperature-sensitive questions, Segrè unfolds a narrative that is at once compelling, surprising, and brilliantly associative. From *Courtesy of Amazon.com. All Rights reserved. www.amazon.com*

"At The Helm: A Laboratory Navigator", by Kathy Barker. Cold Spring Harbor Laboratory (2002) This vigorous, well-organized text provides scientists with the basic management skills they need to lead projects and plan their time. Barker, who is with a private research institution in Seattle, interviewed principal investigators and others in various labs, peppering the text with their quotes as well as material from management sources. Among the topics treated here are hiring practices, time management, how to keep research central, organization, communication, and how to be a leader. From *Book News, Inc.*®, Portland, OR

"Hepatitis B: The Hunt for a Killer Virus", by Baruch S. Blumberg. Princeton Univ Press (2002). Baruch Blumberg, Nobel-prize winner for his discovery of the hepatitis B virus, has never before woven all the strands of the story into a full tapestry. What makes the story doubly fascinating is the worldwide public health importance of hepatitis B, as much of a killer as AIDS. Blumberg is an eloquent writer giving a fascinating account. General readers and experts alike will find this an enjoyable book, not least for the vivid touches that feel first-hand. Jenny Stanton, History Group, London School of Hygiene and Tropical Medicine. From the book jacket.

"An Introduction to Particle Accelerators", by E. J. N. Wilson, Oxford University Press, August, 2001. Wilson, Head of the CERN Accelerator School in Geneva provides graduate students of engineering or physics with an understanding of the physics of large and small accelerators, with the goal of getting them on the right track rather than taking them on the whole journey. He discusses history, designing the patterns of bending and focusing magnets of a synchrotron, maintaining a stable circulating beam, accelerating particles to a high energy, and how to reach the highest possible intensity despite instabilities. He also surveys existing colliders, their applications, and prospects for creating new kinds of accelerators. He includes answers to the exercises. From *Book News, Inc.*®, Portland, OR

"Quantum Optics in Phase Space", by Wolfgang P. Schleich, John Wiley & Sons, February, 2001. Quantum Optics in Phase Space provides an introduction to the rapidly moving field of quantum optics from the point of view of phase space. Modern in style and didactically skillful, it prepares students for their own research by presenting detailed derivations, many illustrations and a large set of workable problems at the end of each chapter. Often, the theoretical treatments are accompanied by the corresponding experiments. An exhaustive list of references provides a guide to the literature. *Quantum Optics in Phase Space* also serves advanced researchers as a comprehensive reference book. Topics extensively discussed include optical interferometry, the atom-field interaction, quantum state preparation and measurement, entanglement, decoherence, the one-atom maser and atom optics in quantized light fields. This is a remarkably concise yet comprehensive and accessible textbook - an inspiring source of information and insight for students, teachers and researchers alike.*Courtesy of Amazon.com. All Rights reserved. www.amazon.com*

"Beethoven's Anvil: Music in Mind and Culture", by William L. Benzon. Hardcover: Basic Books; (2001); paperback: October, 2002. Why does the brain create music? In Beethoven's Anvil, cognitive scientist and jazz musician William Benzon finds the key to music's function in the very complexity of musical experience. Music demands that our symbol-processing capacities, motor skills, and emotional and communicative skills all work in close coordination-not only within our own heads but with the heads (and bodies) of others. Music is at once deeply personal and highly social, highly disciplined and open to emotional nuance and interpretation. It's precisely this coordination of different mental functions, Benzon argues, that underlies our deep need to create and participate in music. *Courtesy of Amazon.com. All Rights reserved. www.amazon.com*

"The Statistical Mechanics of Financial Markets", by Johannes Voit. Springer Verlag; (2001). Describes parallels between physics and finance, including established parallels from the last century, and new research results on capital markets using statistical physics. Discusses the underlying assumptions using empirical financial data, formulating theories of derivative pricing and risk control. *Courtesy of Amazon.com. All Rights reserved. www.amazon.com*

" Crystals and Life: A Personal Journey" by Celerino Abad Zapatero International University Line; ISBN: 0972077405; (September 2002) The book comprises 27 essays grouped within: Basic Elements of Crystallography; Symmtetry and Properties of Protein Crystals; From Data to Electron Density Maps; Protein Structure, Model Building and Refinement; New Technologies; and Future Perspectives. But the resemblance to

a textbook ends there. The essays themselves are masterfully written excursions of fancy given intriguing titles such as "These Naughty, Naughty X-rays," "Can Crystals Cry?', "The Combs of the Wind: Unweaving the X-ray Rainbow," "Only Refined Structures Go to Heaven", "Cathedrals and Synchrotrons for the 21st Century" and "The 1.8Å Structure of Scientific Revolutions." They are laced with historical anecdotes, references to family and Spain, allusions to music and poetry, personal encounters and tributes, and countless similes and metaphors. They are authoritative, but yet they have an easy conversational style. Cele Abad-Zapatero is a romantic and a visionary. His keen observations and fabulous cultural repertoire truly do breathe life into crystals. His colorful book will fascinate anyone interested in nature and discovery. More importantly, it is must reading for crystallographers. Armed thereby with Cele's images and analogies, we will each merge better prepared to communicate the crystallographic story.

Comments by Wayne Hendrickson

"From Semiconductors to Proteins: Beyond the Average Structure (Fundamental Materials Research)" by S. J. L. Billinge & M. F. Thorpe (Editors). Plenum Pub Corp; ISBN: 0306472392; (March 2002) This workshop brought together researchers from materials science, physics, chemistry and biochemistry with interests in determining the structure of substances beyond their average crystal structure. Materials where this is important range from semiconductor alloys to proteins in solution. The workshop featured pedagogical talks on the analysis of diffuse scattering from single crystals and powders, XAFS, NMR, small angle scattering and other techniques which reveal additional information about materials beyond that obtained by Bragg analysis. Theory plays a special role in such studies because of the difficulty of extracting and interpreting information from these techniques. *Courtesy of Amazon.com. All Rights reserved. www.amazon.com*

"Underneath the Bragg Peaks: Structural Analysis of Complex Materials" by T. Egami, S. J. L. Billinge. Elsevier Science Ltd; ISBN: 0080426980; (December 2002) - watch this space for a review in the *Spring Newsletter.*

"No Time to Be Brief: A Scientific Biography of Wolfgang Pauli", by Charles P.Enz. Oxford Univ Press; (September, 2002). Retraces the life ofthe physicist Wolfgang Pauli, analyzes his scientific work, and describes the evolution of his thinking. Pauli spent 30 years as a professor at the Federal Institute of Technology ETH in Zurich, which occupies a central place in this biography. It would be incomplete, however, without a rendering of Pauli's sarcastic wit and, most importantly, of the world of his dreams. It is through the latter that quite a different aspect of Pauli's life comes in, namely his association with the psychology of C.G. Jung and his school.*Courtesy of Amazon.com. All Rights reserved. www.amazon.com*

"The Basics of Crystallography and Diffraction", 2nd Edition, by ChristopherHammond. Oxford Univ Press, (2001- hardcopy and paperback). A hclassic textbook providing a clear and comprehensive introduction to the topic of crystallography and diffraction for undergraduate and beginning graduate students and lecturers in physics, chemistry, materials and earth sciences. For this second edition the existing material has been thoroughly updated. From *Book Description* listed by Oxford University Press.

"***Crystal Growth Technology***", K. Byrappa & T. Ohachi (editors) : 2003 (available December 2002) ISBN:0-8155-1453-0, William Andrew Publishing (Co-published with Springer-Verlag) This book deals with almost all the modern crystal growth techniques that have been adopted, including appropriate case studies. Since there has been no other book published to cover the subject after the Handbook of Crystal Growth, Eds. DTJ Hurle, published during 1993-1995, this book will fill the existing gap for its readers. The book begins with "Growth Histories of Mineral Crystals" by the most senior expert in this field, Professor Ichiro Sunagawa. The next chapter reviews recent developments in the theory of crystal growth, which is equally important before moving on to actual techniques. After the first two fundamental chapters, the book covers other topics like the recent progress in quartz growth, diamond growth, silicon carbide single crystals, PZT crystals, nonlinear optical crystals, solid state laser crystals, gemstones, high melting oxides like lithium niobates, hydroxyapatite, GaAs by molecular beam epitaxy, superconducting crystals, morphology control, and more. For the first time, the crystal growth modeling has been discussed in detail with reference to PZT and SiC crystals. *From Book Description listed at www.williamandrew.com*

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MARCH 2003

17-21 **ICDD Spring Meeting,** ICDD Headquarters, Newtown Square, PA.

APRIL 2003

9-11 **International Workshop on Hard Synchrotron X-rays for Texture and Strain Analysis:** Hamburg, Germany. *www-hasylab.desy.de/conferences/workshop*

MAY 2003

19-23 **3rd National Chemical Conference:** Chemogolovka, Russia. *www.icp.ac.ru/conference/ncc3*

JUNE 2003

2-6 **Workshop on Synchrotron Radiation in Biological Research** Baton Rouge, LA. *hbellamy@lsu.edu*.

4-15 **High Pressure Crystallography, 34th Crystallographic Course** Erice, Italy. *www.crystalerice.org*. Contact Prof. Andrzej Katrusiak: katran@amu.edu.pl

22-27 **Gordon Research Conference on Thin Film and Crystal Growth Mechanisms**, South Hadley, MA

JULY 2003

14-19 **Gordon Research Conference in Structural Biology**

20-24 **The International Congress of Biochemistry and Molecular Biology**, Toronto, Ontario, Canada, *www.iubmb.2003.org*.

20-24 **15th American Conference on Crystal Growth and Epitaxy**, Keystone, CO, *www.crystalgrowth.org*.

24-26 **2003 Current Trends in Microcalorimetry**, Boston, MA, *www.microcalorietry.com/seminars*

21-26 **Aperiodic-2003**, Belo Horizonte, Brazil.

26-31 **American Crystallographic Association Annual Meeting, ACA 2003**, Covington, KY. **www.che.uc.edu/aca/**

AUGUST 2003

4-8 **Denver X-ray Conference,** Marriott Tech Center Hotel, Denver, CO.

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.

14-1 **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

4-30 **Gordon Research Conference on Bioinformatics: From inference to predictive models**, Queens College, Oxford, UK

SEPTEMBER 2003

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

JUNE 2004

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

Workshop on Advanced Methods in X-ray Diffraction Analysis - May 12-17, 2003

A new release of the XD program for X-ray Charge Density Analysis is planned for the spring of 2003. It will include the TOPXD code as an integral component and eliminate a number of bugs in the old version that have been identified. It will use the new relativistic wave functions for atoms and ions, and thus be suitable for analysis of compounds containing relatively heavy elements.

A workshop on the XD methodology and its background is being organized with the purpose to i) initiate those new in the field of accurate X-ray diffraction in the main methodologies of X-ray Charge Density Analysis, ranging from multipolar modeling to the application of the Quantum Theory of Atoms in Molecules and ii) train more experienced users in the use of the new release of the XD programming package.

A limited number of lectures on the theoretical and experimental aspects of charge density determination by X-ray diffraction will be provided and a series of hands-on tutorial sessions for the program XD will be scheduled. To allow maximal instructor-student interaction a maximum of 40 participants is envisioned.

The workshop is planned for the May 12-17, 2003 period at the Chemistry Department, State University of New York, Buffalo, USA. Specific facilities at the University's supercomputer center (ccr.buffalo.edu) will be reserved for exclusive use of the participants.

The workshop will be co-sponsored by Bruker-AXS, and by the Center for Computational Research at the University, and wil be supported by the Office of the Vice President for Research at the University at Buffalo. Support from the International Union of Crystallography has been applied for.

Registration will be $50 for students and $100 for other participants. It is expected that a limited number of fellowships for travel expenses will be available. Lodging costs will be approximately $36- per night for a room with two beds (no extra charge for double occupancy), to be paid before April 5. In order to properly plan the workshop prospective participants are requested to express their interest by sending an e-mail to Irina Novozhilova at chem9988@acsu.buffalo.edu. In case the workshop is oversubscribed, priority will be given to early applicants, so please let us know about your interest as soon as possible.

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