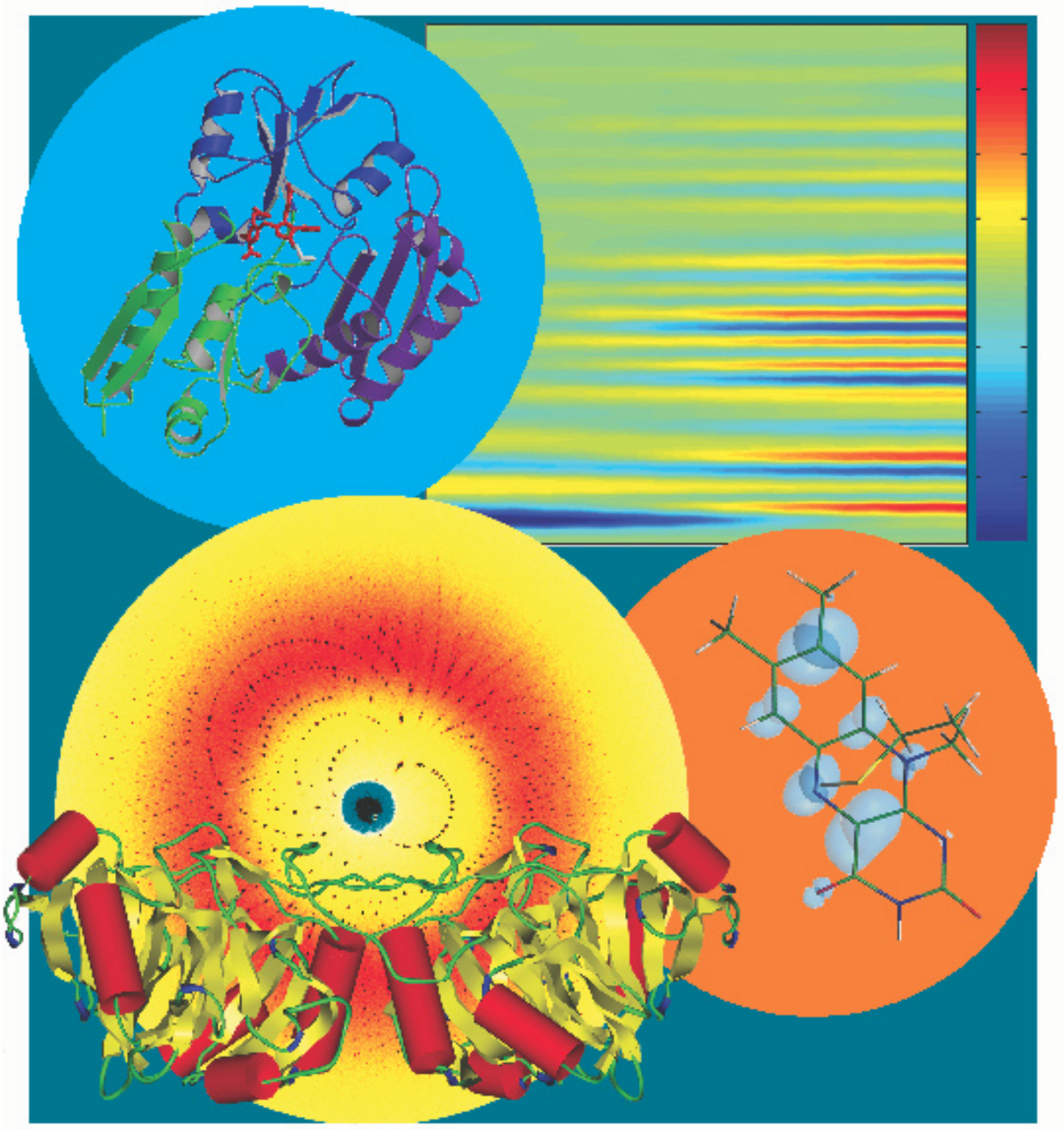
American Crystallographic Association

NEWSLETTER

Number 1 Spring 2003



Time-Resolved Diffraction

Northern Kentucky, July 26-31

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Contributions to the *Newsletter* may be sent to either of the Editors:

Connie Chidester	Judith L. Flippen-Anderson
2115 Glenwood Dr.	3521 Launcelot Way
Kalamazoo, MI 49008	Annandale, VA 22003
tel. 269-342-1600	tel. 703-346-2441
fax 716-852-4846	fax 716-852-4846
conniechidester@earthlink.net	flippen@rscb.rutgers.edu

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

Marcia J. Evans, Administrative Manager
American Crystallographic Association
c/o Hauptman-Woodward Medical Research Institute
73 High Street, Buffalo, NY 14203-0906
phone: 716-856-9600, ext. 321; FAX: 716-852-4846
email: marcia@hwi.buffalo.edu

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

ACA Newsletter (ISSN 1958-9945) Number 1, 2003. Published four times per year in the spring, summer, fall and winter for the membership of the American Crystallographic Association, P.O. Box 96, Ellicott Station, Buffalo, NY 14205-0096. Membership in the ACA includes a non-deductible charge of $1.75 from membership dues to be applied to a subscription to the ACA Newsletter. Periodicals postage paid at Buffalo, New York. POSTMASTER: Send address changes to ACA, c/o 73 High St., Buffalo, NY, 14203.

President's Column

The year 2003 promises to be an exciting and challenging year for ACA, and I look forward to my term as President. One of the nicest benefits of this position is the opportunity for me to become better acquainted with many of ACA's members, as we work together to continue to strengthen the activities of our association. As I have been organizing awards committees and our next nominating committee, I have been greatly gratified by the willingness of our busy members to take on still further work in behalf of ACA; it is this huge volunteer contribution of interest, expertise, and time that makes the ACA run, and makes my association with it such a rewarding experience.

In this vein, I express my gratitude and that of the ACA and its Council to Bill Stallings and Lee Brammer as they leave their posts of Past President and Secretary, respectively. Though we know their dedicated service to ACA will continue, their thoughtful insights at Council discussions will be missed. At the same time, it is my pleasure to welcome newly elected officers Frances Jurnak (as Vice President) and Lisa Keefe (as Secretary) to their posts on ACA Council. I look forward to working with them, and I know you will support them as they contribute their time and efforts to ACA.

While the financial position of ACA is by no means critical, things are tighter everywhere, as we deal with the same trying economic challenges that we face in our personal, business, academic, and government environments. ACA is fortunate to have, both on Council and throughout the association, a large reservoir of expertise and commitment in this arena, and I am confident that ACA will meet its goals of careful stewardship and wise use of our financial resources while we remain true to our core activities and our mission.

ACA awards up for selection this year are the Fankuchen Award (one of ACA's oldest) and the Trueblood Award (to be chosen for the first time). You can read elsewhere in this newsletter the call for nominations for those awards honoring two giants of crystallography (both of whom served as President of our organization). Please note the early deadline for nominations; this will enable the awards committees to make their selections in time for announcement at the 2003 ACA meeting, and so planning can begin for associated symposia for the 2004 meeting in Chicago. The ACA Council is currently reviewing the nominations for the first Margaret C. Etter Early Career Award, which will recognize achievement and future potential among those at an early stage in their independent career.

You have read in the past several newsletters of the strengthening coordination and contact between ACA (as the IUCr regional affiliate for the western hemisphere) and

our Latin American crystallographic colleagues. I invite your attention to the report in this newsletter (p.30) by Iris Torriani (who is also the IUCr representative to the ACA) on the Inter-American Workshop on the Use of Synchrotron Radiation held in Campinas, Brazil in December 2002, in which several of our U.S. colleagues participated. On behalf of Council, I reiterate Past President Charlie Carter's invitation calling attention to the new ACA fund to help provide partial support for attendance at ACA meetings by Latin American crystallographers (as well as to the other worthwhile funds that ACA members have been so generous in establishing and supporting.)

One big thing we have on our collective horizon is the annual ACA meeting, to be held this July 26-31 in Northern Kentucky/ Cincinnati. Jeanette Krause Bauer's program committee has organized a tightly interlocking schedule of sessions, symposia, and workshops that constitute the scientific centerpiece of our gathering. Both the breadth and the focus of the scientific content of our meetings get better and better, as the ACA SIGs take on a large responsibility for planning and organizing sessions and symposia. And the local committee, headed by Bobby Barnett, has arranged for great facilities and a firm infrastructure for our many activities, both scientific and social, (including, of course, the annual banquet, and even a riverboat dinner cruise at the end of the meeting). We appreciate the innumerable hours of preparation that Bobby, Jeanette, and their committees have already devoted and will continue to commit through what promises to be one of our finest ACA meetings.

And in very encouraging news, early indications are that the Exhibit Show at the Northern Kentucky/Cincinnati meeting will be both larger and more varied than ever before. This development, along with the report from the Buffalo office that, despite the current general economic and business climate, ACA now has its largest number ever of corporate members, is further indication of the key position of crystallographic endeavors in today's science and technology. We remain grateful to our industrial and corporate colleagues for this continued support of ACA and of crystallography.

I hope to see you in Northern Kentucky in July!

Ray Davis

Guest Editorial: Former ACA President Penelope Codding

Penny with Herb Hauptman at the 2002 "From Genes to Drugs via Crystallography" course in Erice, Italy.

Why do you stop at a traffic light? Is it because you are committed to social justice or because there may be a cop at the light? The *Sigma Xi* publication *Honor in Science* begins with this question and goes on to state that "scientific honesty is vital because there is no cop at the scientific traffic light".

The recent juxtaposition of celebration notices for the 50th anniversary of Watson and Crick's paper on the structure of DNA and reviews of a new biography of Rosalind Franklin, ***Franklin, The Dark Lady of DNA*** by B. Maddox (*Globe and Mail* newspaper, November 23, 2002) prompts me to ponder whether the problem in science is more than a lack of traffic cops. While we observe, and teach our students to observe, the rules and conventions of science, this is not enough to ensure the ethical conduct of research. There are many other forms of misconduct or misdoing that are subtle and not governed by the rules, or in the words of the opening metaphor, not policed by traffic cops. Are we preparing our students for the situations that call for moral judgements - for making decisions that consider conflicting needs or rights, and that affect the welfare of others?

The discovery of the structure of DNA was a signal achievement in science and is rightly celebrated. It is also right to remind ourselves of the dark side of this discovery, that the authors of that important paper had access to Rosalind Franklin's x-ray results on DNA without her knowledge and without acknowledgement; information that played a key role in the 1953 discovery. For those who are debating whether worrying about subtle forms of misconduct matters, it is useful to be reminded that the shadow of the failure to acknowledge Franklin's contribution has lasted as long as the glory of the discovery.

What can we learn from this story? As an educator, I learn that we need to teach our students to identify the ethical considerations embedded within the process of doing science, and to make moral decisions. Our processes require us to make decisions that impinge on the needs and rights of others. These activities begin at the bench with an obligation for careful experimentation and build outward to obligations regarding the treatment of other persons in the research team and, more removed, to responsibility toward people known only through the review processes of science. At its core, science is built on the right to literature that contains experiments that were competently performed and completely reported. (There is no room for sloppiness or systematic one-sidedness, or trimming and cropping of results, no matter how important the publication is to the career of the authors.) For free exchange of ideas and results, we have a right to receive appropriate and complete acknowledgement of each individual's contribution. Do we teach and model the adage, to give credit always - and only - where credit is due? Acknowledgement is not

limited to authorship issues, which often are governed by rules; it is also about acknowledging the ideas of others in committee meetings, oral presentations, and informal discussions.

We also have a right to a fair and unbiased review based only on the merits of our case. The peer review system for publications, grants, and scientific awards and the tenure and promotion procedures in the academy succeed only when the referees are free of conflict of interest and bias, i.e., when they have no financial or personal interest in the outcome of the decision and can make the decision based only on the evidence. Sadly, data indicate that instances of conflict of interest have delayed publication, augmented the referee's citation index by forced addition of references to their own publications, advanced friends preferentially and led to appropriation of ideas or data, including a legal battle that questioned the peer review system (*Science*, 1995, **270,** 1912-1914). This review system also relies, often implicitly, on protection of the confidentiality of the unpublished work and research plans. Unpublished work should not be shared without the authors' permission and the referee should guard against the subconscious incorporation of ideas from reviewed material into his or her work. We must also teach our students that there are ethical dimensions to the informal system of discussion of results, contributions and careers because great harm can be done by casual comments with no evidentiary basis.

The long lasting shadow of the treatment of Rosalind Franklin emphasizes the importance of making, and teaching our students to make, moral decisions about the ethical dimensions of science. Unfortunately this obligation falls on the shoulders of overburdened senior investigators who may have, according to one letter writer to *Science* (2002, **298**, 2328), as little as two hours per day for proper mentoring. Perhaps the ACA can play a role in supporting discussions of ethical decision-making and avoidance of subtle misdoing or by publicizing the availability of web-based materials like the course in teaching moral reasoning developed at the Poynter Center at Indiana University. (**http://www.indiana.edu/~poynter/mr-main.html**).

I started by quoting from the excellent publication for new scientists, *Honor in Science,* from *Sigma Xi*. I will end by giving this society the last word: "what matters is how we behave in the moments when the task is proving more tedious or complicated than we expected, when the reasons for those difficulties appear to be as trivial as they are persistent, when so much hangs on the result and when nobody is watching."

Penelope Codding

Editor's note: see Book section, page 33 for a review of *Franklin, the Dark Lady of DNA*.

ACA 2002 ELECTION RESULTS

Vice-President	**Frances Jurnak**
Secretary	**Lisa J Keefe**

STANDING COMMITTEES

Continuing Education
Katherine Ann Kantardjieff

Data, Standards, and Computing
Robert M Sweet

Communications
Louis Delbaere

SIGs

Biological Macromolecules
Chair-elect: Lesa Beamer
Secretary/Treasurer: Marilyn D Yoder

General Interest
Chair-elect: Alexandre Yokochi
Member-at-Large: Nicholas Silvaggi

Powder Diffraction (ad hoc Committee)
Abraham Clearfield
Alexandre Yokochi
Xiang Ouyang
Joseph Reibenspies

Service Crystallography
Chair-elect: Alicia Beatty
Secretary/Treasurer: James C Fettinger

Small Angle Scattering
Chair-elect: Brent J Heuser
Member at Large: Elena Kondrashkina

Small Molecules
Chair-elect: Charles Campana

Synchrotron Radiation
Chair-elect: Wayne F Anderson

Young Scientist
Chair-elect: Arwen Pearson
Secretary/Treasurer: James Thompson

Letter to the Editor

Thank you for the opportunity to comment further on Brenda Maddox's biography: *Rosalind Franklin, The Dark Lady of DNA*. Space restrictions in *Physics Today* curtailed my comments on several aspects of Maddox's carefully researched biography. Franklin's family allowed Maddox access to Rosalind's personal letters. Maddox uses these and interviews with the family extensively in the first four chapters. Rosalind Franklin's family were Jews whose English lineage dated to 1763. Her great uncle was the first British high Commissioner to Palestine. Her father was a successful banker who endowed and taught at London's 'The Working Man's College'. From her family life she learned to trust her judgments, live modestly, scorn self-indulgence and look after the financial and scientific welfare of younger colleagues. Photographs contributed by family and friends include the usual conference photos and wonderful photos of her climbing in the Alps. These photos record how the same enthusiasm she brought to her research, she carried into her love of the outdoors. She ice climbed, bicycled, danced and socialized. A letter written the March before her death reveals she was hoping to revel in the American west in August. She was a happy, beautiful, successful woman. Maddox traces Rosalind's friendship with Dorothy Crowfoot Hodgkins. A quote from Hodgkins summarizes her agreement with Rosalind's spirit of scientific objectivity and decision to delay publication, "*As Rosalind was necessarily involved in collecting the accurate data on DNA, it was natural of her to postpone model building until her data was complete, and until she had extracted all the information she could that would limit the kind of model she should build*" (page 178). I felt very privileged to be asked within the last few years to review both this biography and Georgina Ferry's biography, *Dorothy Hodgkin: A Life*, Granta Books, London, UK, 1998; ISBN 1-86207-167-5; (review: *Physics Today* **53**, 68 (2000).

Eugenie Vorburger Mielczarek

Editor's note: see page 33 for her book review of *Rosalind Franklin, The Dark Lady of DNA*.

New ACA VP Frances Jurnak

New ACA Vice President

Our newly elected Vice-President this year is Frances Jurnak. In 1968 Fran earned her B.S. in Chemistry from Catholic University of America in Washington D.C. She switched coasts for her doctorate degree, which is also in Chemistry, from the University of California, Berkeley. She received her Ph.D. degree in 1973 from the lab of David Templeton. Fran began with small molecule crystallography, under the mentorship of Kenneth Raymond and David Templeton. She began her transition to macromolecular crystallography as a post-doc in the lab of Alexander Rich at the Massachusetts Institute of Technology. After a second post-doc at the Milton S. Hershey Medical Center, Pennsylvania State University, she accepted a position at the University of California, Riverside in 1979. Since 1997 she has been a Professor in the Department of Physiology and Biophysics at the University of California, Irvine.

At UCI, Fran is very active in graduate program activities. Her involvement has included service as: member of the Admissions Committee; Chair of the Structural Biology track within the larger graduate program; Co-director of Structural Biology within the Comprehensive Cancer Center; Chair of the Graduate Council at UCI; and representative to the UC system wide CCGA (Coordinating Council on Graduate Activities). She is currently serving on the editorial board of the *Journal of Structural Biology.*

I met Fran when I began my Ph.D. studies at the University of California, Riverside. Unlike most of my fellow students, I chose a dissertation advisor not for a research area or experimental technique, but for the scientific knowledge and the person from whom I believed I would learn the most. Fran became my dissertation advisor and it was a decision that I look back on as a wise choice. When I was Fran's student , she encouraged my membership and involvement with the ACA and we continue to meet frequently at ACA meetings.

Fran's lab has studied the elongation factors EF-Tu for many years. Her research efforts have focused on the role of elongation factors in ribosomal protein synthesis as well as their role as chaperones and their protein disulfide isomerase activity during cellular stress. A second research interest involves bacterial pectate and pectin lyases and their homologues in plants.

Please join me in congratulating Fran in her election to the office of Vice President of the ACA. She will serve the Association well.

Marilyn Yoder

ACA Secretary Lisa Keefe

The ACA membership has elected Lisa J. Keefe, Director of IMCA-CAT at the Advanced Photon Source, as our next Secretary. Lisa received an A.B. in Chemistry from Vassar College in 1983 before enrolling in the graduate program in Biophysics and Biophysical Chemistry at the Johns Hopkins University School of Medicine. Lisa worked in Carl Pabo's laboratory at Hopkins through 1989, when she moved to Ed Lattman's laboratory, where she earned her Ph.D. in 1992. She then received a DOE Alexander Hollaender Distinguished Postdoctoral Fellowship with a joint appointment in the Structural Biology Center (SBC) at Argonne National Laboratory and the Biology Department of Brookhaven National Laboratory, where she helped to develop the user program for SBC, first at the National Synchrotron Light Source (Brookhaven) and then at the Advanced Photon Source (Argonne). In 1998 she joined the Industrial Macromolecular Crystallography Association Collaborative Access Team (IMCA-CAT) at the APS as a user interface scientist; she was promoted to User Program Coordinator in 2001, and replaced me as Director of IMCA-CAT in July 2002. She directs the CAT's technical and user programs, and manages the activities of a staff of six. She shares with me the role of Principal Investigator of the contract by which Illinois Institute of Technology manages the IMCA Collaborative Access Team.

I first met Lisa when she was a graduate student at Hopkins and I was at Genex Corporation in nearby Gaithersburg, MD; she struck me as a dynamic and effective crystallographer and biochemist even then. She developed a solid reputation for managing user programs at synchrotron beamlines when she was with SBC, so when John Chrzas and I were building a user-program staff for IMCA-CAT in 1997-98, we recognized that she would be able to make a significant contribution. The pharmaceutical companies that provide the funding and direction for IMCA-CAT decided in early 2002 that the CAT would be most effectively managed by a full-time director rather than a half-time academic like me, and after an open search, they appointed Lisa to the Directorship.

Lisa worked on difficult macromolecular structure problems at Johns Hopkins and at SBC, and she has collaborated with structural biologists from Emory University and other institutions since her arrival at IMCA-CAT. Most of her effort is focused on operating and improving the facilities of the CAT. This involves making the most of the facilities as they exist now, and developing and implementing clear-eyed plans for the future.

Lisa has been active in the APS's activities beyond the walls of IMCA-CAT. She has been a member of the APS User Organization Steering Committee since 2001, and helped to draft and implement the current procedures by which general users obtain access to APS beamlines. She has been a member of the ACA for over a decade, and was chair of the ACA Young Scientists' SIG from 1993 to 1994. Lisa and her husband, fellow APS crystallographer Stephan Ginell of SBC-CAT, have three young children. I hope you will join me in wishing Lisa well in her new ACA responsiblities.

Andy Howard

Lawrence Award to Keith Hodgson

These awards were established in 1959 to honor the memory of Ernest O. Lawrence, who invented the cyclotron, and after whom two major Energy Department national laboratories in Berkeley and Livermore, CA are named. The awards are given by the DOE for outstanding contributions in the field of atomic energy. Each winner received a gold medal, a citation, and $25,000 at a ceremony held in Washington, DC on Oct 28th, 2002.

Keith O. Hodgson, professor of chemistry at Stanford University and Director of the Stanford Synchrotron Radiation Laboratory, was honored in the chemistry category *for his contributions to the development of synchrotron x-rays for the investigation of biological structure and function.* At Stanford, he uses bio-inorganic and biophysical chemistry to investigate how structure at different organizational levels relates to function.

Hodgson graduated from the University of Virginia with a BS in 1969. He continued his studies at the Univ. of CA, Berkeley, where he earned a PhD in 1972. He was a NATO postdoctoral fellow at the Swiss Federal Institute of Technology in Zurich and an Alfred P. Sloan Foundation Fellow before joining the faculty at Stanford.

Brünger and Jones: Gregori Aminoff Prize

The **Gregori Aminoff Prize in Crystallography for 2003** is awarded to **Prof. Axel Brünger,** Stanford University, *"for his development of refinement techniques for macromolecules"* and **Prof. T. Alwyn Jones,** Uppsala University, Sweden, *"for his pioneering development of methods to interpret electron density maps and to build models of biological macromolecules with the aid of computer graphics"*.

The Gregori Aminoff Prize is awarded by the Royal Swedish Academy of Sciences and is intended to reward a documented, individual contribution in the field of crystallography, including areas concerned with the dynamics of the formation and dissolution of crystal structures. Some preference is shown for work evincing elegance in the approach to the problem. The Aminoff Prize was awarded for the first time in 1979. In 2002, the prize amounted to SEK 50 000. The laureates will receive the prize at a ceremony at the Royal Swedish Academy of Sciences in Stockholm on September 10, 2003.

National Lecturer Award to Janet Thornton

The **Biophysical Society 2003 National Lecturer Award** *for excellence and leadership in the biophysical sciences* was presented to **Janet Thornton,** European Bioinformatics Institute at their annual meeting in San Antonio, TX on March 3, 2003.

ACA Council News

Rather than the typical spring, summer and fall meetings, the ACA Council met formally only twice in 2002, once in San Antonio directly prior to the ACA annual meeting and on November 9th in Washington DC.

At the May meeting, the Council approved two new awards named after the late Professor Peggy Etter, one aimed at crystallographers early in their independent career and a second aimed at students. The former will be awarded annually after selection by the ACA Council from nominations received. The first award is expected to be presented at the Covington meeting this summer. The Margaret C. Etter Student Lecturer Awards will provide an opportunity for students selected by each SIG to present lectures in appropriate sessions at the annual ACA meetings, as well as providing a small honorarium. In San Antonio, the ACA Council also met with a group of about 15 crystallographers from Latin and South American countries with a view to developing improved and more formal links between the ACA and crystallographers throughout the Western Hemisphere. This meeting was followed up by a further meeting during the IUCr Congress in Geneva. It was decided that the initial step forward would be to form a Latin and South American Crystallographers SIG.

In Washington DC, the Council met with Andy Howard (Illinois Institute of Technology) to discuss plans for organization of the new ACA Summer School. The school is to be sited in the Chicago area at IIT and Argonne National Laboratory **(see p. 23)**. The ACA budget was discussed extensively with the focus on ways and means of establishing necessary increases in revenue without unduly increasing the burden on the membership. Future meeting sites were discussed at length, with sites in the southeastern USA under consideration for 2005 and sites in Canada being examined for 2006 or 2007. With respect to Canadian members the issue of providing a means for donations to be tax-deductible in Canada was discussed and will be investigated. The Council also approved a petition to initiate a new SIG on Structure Determination from Powder Diffraction, which has been spearheaded by Abe Clearfield (Texas A&M University). **(See p. 9.)**

On a personal note, my term of office as member of the ACA Council is now at an end and I wish Lisa Keefe well as she takes over as Secretary. I have enjoyed my three years on the Council. I have also found it very interesting to be involved in the running of the organization and I would certainly encourage others to get involved. Participation is ultimately what keeps organizations like the ACA thriving for the benefit of all its members.

Lee Brammer, (former) Secretary, ACA

News from Canada:

January, 2003

1. ***The Canadian National Committee of the IUCr*** met on January 11th in Montreal. The Committee currently consists of Suzanne Fortier (Chair), Joe Schrag (Secretary), J.P. Charland (Treasurer), Stan Cameron, Frank Hawthorne, Francois Brisse and David Rose (ex officio). The committee was joined by the Canadian Delegates to the Geneva IUCr, Louis Delbaere, David Brown and George Ferguson. We were happy to welcome our special guest, Bill Duax, President of the IUCr, who generously took the time to join us, and gave his perspective on upcoming issues on the international scene.

One of the many items discussed was the possibility of setting up a travel fund for Canadian students to attend ACA meetings. A proposal is being drafted. Watch this space!

Another discussion concerned the awards of **Canada Research Chairs** to members of the crystallographic community.

2. ***CanadaQuirks: CANADA RESEARCH CHAIRS***

*(In the **CanadaQuirks** section, your correspondent attempts to clarify Canadian terms, organizations, issues, etc. that might be of interest to the crystallographic community.)*

There has been a move by the federal government to increase spending in research and development, and much of this increase has been targeted to specific high-profile programs. One such program is the Canada Research Chairs. In 2000, the Government introduced this funding to support as many as 2000 Chairs by 2005 in Universities across the country. There have been two rounds of Chairs awarded, in 2001 and 2002. The primary objectives are recruitment of promising and/or established scientists from abroad (reverse brain-drain) and retention of top scientists within Canada. Secondly, the program, unlike many in Canada, will provide some level of resources towards institutional (indirect) costs.

There are two types of Chairs. "Tier I" Chairs are judged to be international leaders in their fields and are awarded 7-year renewable Chairs. "Tier II" Chairs, which have a renewable 5-year term, are geared towards young scientists who have the potential to be leaders in their fields. The fields represented by the Chairs are extremely broad, covering Social Science, Natural Science and Engineering, and Health Research.

A list of Chair holders in the crystallography/diffraction community includes: **Louis Delbaere** (Saskatchewan), **Albert Berghuis** (McGill), **Z. Jia** (Queen's), **Emil Pai** (Toronto), **Frank Hawthorne** (Manitoba), **Mike James** (Edmonton), **Mark Glover** (Edmonton), **Adam Hitchcock** (McMaster) and **T.K. Sham** (Western Ontario). Sincere apologies to any who might have been missed. Further information, including a full list of Chair holders, is at **www.chairs.gc.ca.**

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

David Rose, Canadian Representative to ACA Council

Call for Nominations for Fankuchen and Trueblood Awards

Nominations are solicited for the 2004 **Fankuchen Memorial Award** and for the **Kenneth N. Trueblood Award**. Both awards will be presented at the annual ACA meeting in Chicago in July, 2004. The recipients will give their lectures at the special Fankuchen and Trueblood Award Symposia organized to honor them. Both awards are given every three years and each consists of an honorarium plus travel expenses to accept the award. There are no geographic or age restrictions. The Fankuchen Award carries the additional responsibility that the Award Lecture should also be presented at an academic institution of the recipient's choice. Please submit nominations to the ACA office in Buffalo (see page 1 for address) no later than June 1, 2003. A nominating letter clearly indicating the accomplishments of the individual is required; an additional supporting letter and a c.v. for the nominee may be provided, but are not required.

The **Fankuchen Award** was established in 1971 in memory of Isidor Fankuchen, Professor of Physics at the Polytechnic Institute of Brooklyn from 1942 to 1964. It is given to recognize contributions to crystallographic research by one who is known to be an effective teacher of crystallography. Previous winners were: **2001: James Stewart; 1998: E. Dodson; 1995: Jenny Glusker and Kennth Trueblood; 1992: L. D. Casper; 1989: David Sayre; 1986: Michael S. Rossmann; 1983: Lyle H. Jensen; 1980: David Harker; 1977: Dorothy Hodgkin; 1974: A. Guinier; 1971: Martin J. Buerger.**

The first **Kenneth N. Trueblood Award** will be given in 2004. It was created to recognize exceptional achievement in computational or chemical crystallography. The award was established in 2001 in memory of Professor Kenneth N. Trueblood, UCLA 1949-1998, who was a major force in the early use of computers and the development of crystallographic computer programs. He applied these programs to the examination of chemical and molecular details of many structures at the frontiers of research. His contribution to the famous work on vitamin B12 is one example. Professor Trueblood was a leader in the development of techniques for analysis of anisotropic motion and was also a superb teacher and a lucid author. The award will be given every three years and consists of an honorarium plus travel expenses to accept the award. The award selection committees are:

Fankuchen: **Hugo Steinfink, Abe Clearfield, Joel Oliver and Marilyn Olmstead**

Trueblood: **Jenny Glusker, Bryan Craven, Katherine Kantardjieff, and Bobby Barnett**

Desiraju is made TWAS Fellow

Prof. G. R. Desiraju, University of Hyderabad, India, was recently elected as a Fellow of the Third World Academy of Sciences (TWAS). TWAS, with headquarters in Trieste, is an association for the promotion of scientific excellence for sustainable development in the Third World. Forty-three new fellows were elected in October 2002, of which four were in the area of chemical sciences.

ICDD Announces Ludo Frevel Scholarships

From 34 commendable applications, the ICDD Ludo Frevel Crystallography Scholarship Committee has selected 6 to receive scholarships in 2003:

Kacey Claborn, University of Washington, Seattle, with research involving *Measurement of Optical Rotation in the Achiral Crystals of Pentaerythritol.*

Sean Dalrymple, University of Calgary, Calgary, Alberta, CA, with exploration into *Flexible Hydrogen Bonded Networks via Second Sphere Coordination.*

Desiree Fong, McGill University, Montreal, Quebec, CA with major interest in *Substrate Binding Properties and Reaction Mechanism of an Aminoglycoside-Modifying Kinase.*

Erwann Jeanneau, University of Rennes, Rennes, France with studies focusing on *Design of New Mixed Oxalates With Open-Framework Structures Based on MO8 Building Units.*

Chong Lim, University of Illinois at Urbana-Champaign, Urbana IL with research concerning *Crystallographic and Structural Studies of Cobalt Silicide Formation on Si(001).*

Andrew Locock, University of Notre Dame, South Bend, IN, who is investigating *Crystal Structure and Synchrotron Radiation Study of Uranyl Oxysalts of Phosphate and Arsenate-Implications for Remediation.*

Each student will receive $2,250, to assist in the continuation of studies in crystallography. Awards are made possible by donations from both individuals and corporations to the Ludo Frevel Crystallography Scholarship Fund which was established to assist aspiring student crystallographers in their research. Direct contributions to: Crystallography Scholarship Fund, ICDD, 12 Campus Blvd., Newtown Square, PA 19073.

Announcing New Powder Diffraction SIG

A new Special Interest Group will come into being at the Northern Kentucky 2003 ACA meeting. During the 2002 ACA meeting in San Antonio a petition was circulated to that effect and the requisite number of signatures was obtained. Those who attended the *Transactions Symposium* at the San Antonio meeting on *Crystal Structure Determination from Powder Diffraction Data* were treated to an overview of how sophisticated the methodology and software has become. With the growing need and the increasing number of structures solved from powder diffraction data, it is essential that such techniques become another tool in the crystallographer's arsenal. The Powder Diffraction SIG will be the focal point in disseminating information on advances in powder based structure solutions and in presenting the latest results at our national meetings. We have planned a half day session for the upcoming ACA meeting in Northern Kentucky and will hold a business meeting to elect officers and ratify a constitution. All who are interested are welcome.

Abe Clearfield

ACA COUNCIL OFFICERS - 2003

PRESIDENT

Raymond E. Davis
Dept. of Chemistry & Biochemistry
The Univ. of Texas at Austin
Austin, TX 78712-1167
(512) 471-4440
Fax (512) 471-8696
redavis@mail.utexas.edu

VICE PRESIDENT

Frances Jurnak
Dept of Physiology & Biophysics
Medical Sciences I D 350
Univ. of California, Irvine
Irvine CA 92697-4560
(949) 824-6623
Fax: (949) 824-8540
jurnak@uci.edu

PAST PRESIDENT

Charles W. Carter, Jr.
Dept. of Biochemistry & Biophysics
CB7260
Univ. of North Carolina
Chapel Hill, NC 27599-7260
(919) 966-3263
Fax (919) 966-2852
carter@med.unc.edu

TREASURER

Douglas Ohlendorf
Dept. of Biochemistry
Molecular Biology & Biophysics
6-155 Jackson Hall
Univ. of Minnesota
Minneapolis, MN 55455
(612) 624-8436
Fax (612) 624-5121
ohlen@umn.edu

SECRETARY

Lisa J. Keefe
IMCA-CAT, Sector 17, Bldg. #435A
Advanced Photon Source
Argonne National Laboratory
9700 South Cass Ave.
Argonne, IL 60439
(630) 252 0544
Fax: (630) 252 0521
keefe@anl.gov

CANADIAN REPRESENTATIVE

David Rose
Ontario Cancer Institute
610 University Ave.
Toronto, Ontario
Canada M5G 2M9
(416) 946-2970
Fax (416) 946-6529
drose@oci.utoronto.ca

APPOINTMENTS

FINANCIAL OFFICER

S.N. Rao
College of Graduate Studies & Research
Room 404, University Center
Univ. of Central Oklahoma
100 N. University Dr.
Edmond, OK 73034-5209
(405) 974-2524
Fax (405) 974-3852
srao@ucok.edu

EXECUTIVE OFFICER

William L. Duax
Hauptman Woodward Medical Res. Inst.
73 High St.
Buffalo, NY 14203-1196
(716) 856-9600 ext. 308
Fax: (716) 852-4846
duax@hwi.buffalo.edu

IUCr REPRESENTATIVE

Iris L. Torriani
Inst. De Fisica
Univ. Estadual de Campinas
C.P. 6165
13083-970 Campinas SP, Brazil
55 19 3788 5497
Fax: 55 19 3289 3137
torriani@ifi.unicamp.br

ADMINISTRATIVE MANAGER

Marcia Evans
ACA
P.O. 96 Ellicott Station
Buffalo, NY 14205-0096
(716) 856-9600 ext. 321
Fax: (716) 852-4846
marcia@hwi.buffalo.edu

NEWSLETTER EDITORS

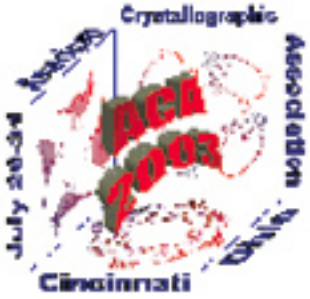
Judith Flippen-Anderson
3521 Launcelot Way
Annandale, VA 22003
(703) 560-7436
Fax: (716) 852-4846
flippen@rcsb.rutgers.edu

Connie Chidester
2115 Glenwood Dr.
Kalamazoo, MI 49008
(269) 342-1600
Fax: (716) 852-4846
conniechidester@earthlink.net

CANADIAN DIVISION

Gary Enright, *Chair*
Steacie Inst. For Molecular Sciences
National Research Council of Canada
Ottawa, Ontario
Canada K1A 0R6
(613) 993-7393
gary.enright@nrc.ca

Brian Patrick, *Secretary*
Chemistry Dept.
Univ. of British Columbia
Vancouver, British Columbia
Canada V6T 1Z1
(604) 822-4865
brian@xray5.chem.ubc.ca



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STANDING COMMITTEES 2003

Communications

John S. Sack (03)
Bristol-Myers Squibb
P.O. Box 4000, H23-03
Princeton NJ 08543-4000
Tel: 609 252 5559
Fax: 609 252 6030
john.sack@bms.com

Jeanette A. Krause Bauer (04)
Dept. of Chemistry
Univ. of Cincinnati
PO Box 210172
Cincinnati, OH 45221-0172
Tel: 513 556 9226
Fax: 513 556 9239
jeanette.krause@uc.edu

Kay Onan (05)
Office of the President
Northeastern Univ.
Boston, MA 02115
Tel: 617 373 2101
Fax: 617 373 5015
k.onan@nunet.neu.edu

Louis Delbaere (06)
Dept of Biochemistry
Univ. of Saskatchewan
107 Wiggins Rd.
Saskatoon SASK S7N 5E5
Canada
Tel. 306 966 4360
Fax: 306 966 4390
louis.delbaere@usask.ca

Continuing Education

Winnie Wong-Ng (03)
Materials Sci & Eng Lab
NIST
Bldg 223 Rm A256
Gaithersburg, MD 20899
Tel: 301 975 5791
Fax: 301 975 5334
winnie.wong-ng@nist.gov

Phillip Fanwick (04)
Dept of Chemistry
Purdue Univ.
Brown Lab
West Lafayette IN 47907-1393
Tel: 765 494 4572
Fax: 765 494 0239
fanwick@xray.chem.purdue.edu

Marilyn M. Olmstead (05)
Dept of Chemistry
Univ. of California Davis
One Shields Ave.
Davis, CA 95616-5295
Tel: 530 752 6668
Fax: 530 752 8995
olmstead@indigo.ucdavis.edu

Katherine Ann Kantardjieff (06)
Dept of Chemistry & Biochemistry
Calif State Univ. Fullerton
800 N State College Blvd.
Fullerton, CA 92834
Tel: 714 278 3752
Fax: 714 278 5316
kkantardjieff@fullerton.edu

Data, Standards & Computing

John C. Huffman (03)
Dept of Chemistry
Indiana Univ.
Bloomington IN 47405
Tel: 812 855 6742
Fax: 812 855 8300
huffman@indiana.edu

Helen M. Berman (04)
Chemistry/Wright & Rieman Labs
Rutgers Univ.
610 Taylor Rd.
Piscataway, NJ 08855-0939
Tel: 732 445 4667
Fax: 732 445 4320
berman@rcsb.rutgers.edu

Jeffrey R. Deschamps (05)
Structure of Matter Code 6030
Naval Research Lab
4555 Overlook Ave SE
Washington, DC 20375
Tel: 202 767 0656
Fax: 202 767 6874
deschamps@nrl.navy.mil

Robert M. Sweet (06)
Biology Dept
Brookhaven Nat'l Lab
Upton NY 11973
Tel: 631 344 3401
Fax: 631 344 3407
sweet@bnl.gov

SPECIAL INTEREST GROUP OFFICERS

Biological Macromolecules

Vivien C Yee, Chair (03)
Molecular Cardiology/NB20
Cleveland Clinic Foundation
9500 Euclid Ave.
Cleveland OH 44195
Tel: 216 444 2057
Fax: 216 445 1466
yeev@ccf.org

Lesa Beamer, Chair-elect (04)
Dept. of Biochemistry
Univ. of Missouri Columbia
117 Schweitzer Hall
Columbia MO 65211
Tel: 573 882 6072
Fax: 573 884 4812
beamerl@missouri.edu

Marilyn D Yoder - Sec./Treas. (04)
Univ. of Missouri-Kansas City
5100 Rockhill Rd
Kansas City MO 64110-2499
Tel: 816 235 1986
Fax: 816 235 1503
yoderm@umkc.edu

Fiber Diffraction

Thomas C Irving, Chair (03)
Biochemistry, Physical Sciences
Illinois Inst. of Technology
3101 S Dearborn
Chicago IL 60616
Tel: 312 567 3489
Fax: 312 567 3494
irving@biocat1.iit.edu

Jennifer Taylor, Sec./Treas. (04)
Dept. of Materials Science
Univ. of Cambridge
Pembroke St.
Cambridge, CBZ 3QZ UK
Tel: 44 1223 762 866
Fax: 44 1223 334 567
jet50@cam.ac.uk

General Interest

Hugo Steinfink, Chair (03)
Dept. of Chemical Engineering
Univ. of Texas Austin
Austin TX 78712
Tel: 512 471 5233
Fax: 512 471 7060
steinfink@che.utexas.edu

Alexandre Yokochi, Chair-elect (04)
Dept. of Chemistry
Oregon State Univ.
Corvallis OR 97331
Tel: 541 737 6724
Fax: 541 737 2062
alex.yokochi@orst.edu

Vivian Cody, Sec./Treas. (03)
Hauptman-Woodward MRI
73 High St
Buffalo NY 14203-1196
Tel: 716 856 9600 ext 322
Fax: 716 852 6086
cody@hwi.buffalo.edu

Nicholas Silvaggi,
Member at Large (04)
Dept. of Molecular & Cell Biology
Univ. of Connecticut
75 N Eagleville Rd
Storrs CT 06269
Tel: 860 486 2099
Fax: 860 486 4331
nicholas.silvaggi@huskymail.uconn.edu

Materials Science

Charlotte Lowe Ma, Chair (03)
Res & Advanced Engineering
Ford Motor Company
MD 3083 SRL
PO Box 2053
Dearborn, MI 48121-2053
Tel: 313 317 7382
Fax: 313 322 7044
clowema@ford.com

Richard L Harlow, Sec./Treas. (03)
7 Shull Dr Devon
Newark DE 19711
Tel: 302 695 2097
Fax: 302 695 1351
rharlow@conectiv.net

Neutron Scattering

Thomas Proffen, Chair (03)
Los Alamos Nat'l Lab
LANSCE-12, MS H805
Los Alamos NM 87545
Tel: 505 665 6573
Fax: 505 665 2676
tproffen@lanl.gov

James W Richardson, Sec./Treas. (03)
IPNS Div.
Argonne Nat'l Lab
9700 S Cass Ave.
Argonne IL 60439
Tel: 630 252 3554
Fax: 630 252 4163
jwrichardson@anl.gov

Powder Diffraction

(ad hoc Powder SIG committee)

Abraham Clearfield
Dept. of Chemistry
Texas A & M Univ.
PO Box 30012
College Station TX 77843-3255
Tel: 979 845 2936
Fax: 979 845 2370
clearfield@mail.chem.tamu.edu

Alexandre Yokochi
Dept. of Chemistry
Oregon State Univ.
Corvallis OR 97331
Tel: 541 737 6724
Fax: 541 737 2062
alex.yokochi@orst.edu

Xiang Ouyang
Dept. of Chemistry
Texas A & M Univ.
College Station TX 77843
Tel: 979 845 3812
ouyang@mail.chem.tamu.edu

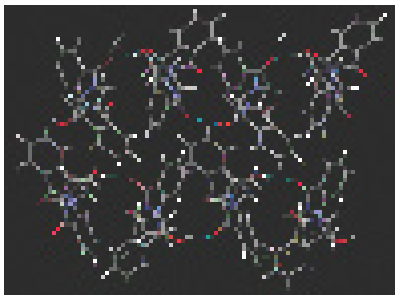
Joseph Reibenspies
Dept. of Chemistry
Texas A & M Univ.
College Station TX 77843-3255
Tel: 979 845 9125
Fax: 979 845 8184
reibenspies@mail.chem.tamu.edu

Service Crystallography

Richard J Staples, Chair (03)
Dept. of Chemistry
Harvard Univ.
12 Oxford St.
Cambridge MA 02138
Tel: 617 495 0787
Fax: 617 496 5618
staples@chemistry.harvard.edu

Alicia Beatty, Chair-elect (04)
Dept. of Chemistry and Biochemistry
Univ. of Notre Dame
251 Nieuwland Science Hall
Notre Dame IN 46556-5670
Tel: 574 631 5935
Fax: 574 631 6652
abeatty@nd.edu

James C Fettinger, Sec./Treas.(04)
Dept. of Chemistry Room B0117
Univ. of Maryland
College Park MD 20742
Tel: 301 405 1861
Fax: 301 314 9121
jf96@umail.umd.edu



250,000th entry in the CSD, Isoindolo (2,1-a)pyrrolidino(2,1-c)(1,4)benzodiazepine-1,12-dione-6-ol,*Angewandte Chemie (Int'l Edition)*, 2001, 40, 577-579; A.G. Griesbeck, W. Kramer, J. Lex. *From CCDC website:* http://www.ccdc.cam.ac.uk

Small Angle Scattering

Jinkui Zhao, Chair (03)
Spallation Neutron Source
Oak Ridge Nat'l Lab
701 Scarboro Rd.
Oak Ridge TN 37830
Tel: 865 574 0411
Fax: 865 241 5177
zhaoj@oml.gov

Brent J Heuser, Chair-elect (04)
Dept. of Nuclear Engineering
Univ. of Illinois
103 S Goodwin Ave.
Urbana IL 61801-2984
Tel: 217 333 9610
Fax: 217 333 2906
bheuser@uiuc.edu

Pete Jemian, Sec./Treas.(03)
Mar Research Lab
Univ. of Illinois
9700 S Cass Ave.
Argonne IL 60439
Tel: 630 252 0863
Fax: 630 252 0862
jemian@anl.gov

Elena Kondrashkina, Member at Large (04)
Dept. Bio. Chem. & Physi Sci
Illinois Inst. of Technology
9700 S Cass Ave. Bldg. 435B
Argonne IL 60439
Tel: 630 252 0508
Fax: 630 252 0545
elena@bio.aps.anl.gov

Synchrotron Radiation

James F Fait, Chair (03)
SER-CAT
34 Kentland Dr.
Romeoville, IL 60446
Tel: 630 252 0644
Fax: 630 252 0641
fait@anl.gov

Wayne F Anderson, Chair-elect (04)
Mol Pharm & Biochemistry
Northwestern Univ. Medical School
303 E Chicago Ave.
Chicago IL 60611
Tel: 312 503 1697
Fax: 312 503 5349
wf-anderson@northwestern.edu

Small Molecules

Brian Patrick, Chair (03)
Dept. of Chemistry
Univ. of British Columbia
2036 Main Mall
Vancouver BC V6T 1Z1 CANADA
Tel: 604 822 4865
bpatrick@chem.ubc.ca

Charles Campana, Chair-elect (04)
Bruker Nonius
5465 E Cheryl Pkwy.
Madison WI 53711-5373
Tel: 608 276 3042
Fax: 608 276 3006
ccampana@bruker-axs.com

Joseph Reibenspies, Sec./Treas. (03)
Dept. of Chemistry
Texas A & M Univ.
College Station TX 77843-3255
Tel: 979 845 9125
Fax: 979 845 8184
reibenspies@mail.chem.tamu.edu

Young Scientists

C Kent Brown, Chair (03)
Dept. of Biochemistry
Univ. of Minnesota
321 Church St.
Minneapolis MN 55455
Tel: 612 625 5175
brow0927@tc.umn.edu

Arwen Pearson, Chair-elect (04)
BMBB
Univ. of Minnesota
6-155 Jackson Hall
321 Church St
Minneapolis MN 55455
Tel: 612 624 0141
Fax: 612 624 5121
pears079@umn.edu

James Thompson, Sec./Treas. (04)
6124 45th Ave. N
Crystal MN 55422
Tel: 612 625 2115
Fax: 612 625 2163
thompson@dcmir.med.umn.edu

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Contributors to This Issue:

Ray Davis, Penelope Codding, Marilyn Yoder, Andy Howard, Lee Brammer, David Rose, Abe Clearfield, James Raftery, John Helliwell, Seol Ryu, Richard Stratt, Peter Weber, Roman Federov, Ilme Schlichting, Andrew Mesecar, John Sack, Bryan Craven, Charles Lake, Cele Abad-Zapatero, John Faber, Iris Torriani, Eugenie Mielczarek, Helen Berman, Alex Chernov, Bobby Barnett, Jeanette Krause Bauer, Bernie Santarsiero, Karl Volz, Christer Aakeröy

Chair

JON CLARDY (05)
Harvard Medical School, BCMP
240 Longwood Avenue
Boston, MA 02115
Phone: 617-432-2845
Fax: 617-432-3702
jon_clardy@hms.harvard.edu

Vice-Chair

JAMES A. KADUK (05)
BP Chemicals
150 W. Warrensville Road
P.O. Box 3011, MC F-9
Naperville, IL 60566
Phone: 630-420-4547
Fax: 630-420-5252
kadukja@bp.com

Secretary-Treasurer

WINNIE WONG-NG (03)
Ceramics Division
NIST
Bldg. 223 Room 256
Gaithersburg, MD 20899
Phone: 301-975-5791
Fax: 301-975-5334
winnie.wong-ng@nist.gov

Members

PHILIP E. BOURNE (05)
Integrative Biosciences San Diego Supercomputer Center
University of California, San Diego
9500 Gilman Drive
La Jolla, CA 92093-0537
Phone: 858-822-8301
Fax: 858-822-0873
bourne@sdsc.edu

JOEL D. BROCK (04)
Applied and Engineering Physics
Cornell University
210A Clark Hall of Science
Ithaca, NY 14853–2501
Phone: 607-255-0639
Fax: 607-255-7658
jdb20@cornell.edu

HOWARD M. EINSPAHR (03)
67 Green Avenue
Lawrenceville, NJ 08648-1623
Phone: 609-844-0664
hmeinspahr@yahoo.com

KEN DOWNING (05)
Lawrence Berkeley National Laboratory
1 Cyclotron Road Mail Stop 1-0112
Berkeley, CA 94720
Phone: 510-486-5941
Fax: 510-486-6488
KHDowning@lbl.gov

KATHRYN R. ELY (03)
Program on Molecular Assemblies and Cell Structure
The Burnham Institute
10901 N. Torrey Pines Rd.
La Jolla, CA 92037-1062
Phone: 858-646-3135
ely@burnham.org

KATHERINE A. KANTARDJIEFF (03)
Dept. of Chemistry and Biochemistry
California State University, Fullerton
800 N State College
Fullerton, CA 92834-9480
Phone: 714-278-3752
Fax: 734-939-4225
kkantardjieff@fullerton.edu

PETER KUHN (04)
The Scripps Research Institute
Scripps PARC Institute, CB227
10550 N. Torrey Pines Road
La Jolla, CA 92037
Phone: 858-784-9114
Fax: 858-246-5054
pkuhn@scripps.edu

MARILYN M. OLMSTEAD (04)
Department of Chemistry
University of California, Davis
One Shields Ave
Davis, CA 95616–5295
Phone: 530-752-6668
Fax: 530-752-8995
olmstead@indigo.ucdavis.edu

JOHN PARISE (05)
Department of Geosciences
State University of NY Stony Brook
Stony Brook, NY 11794-2100
Phone: 631-632-8196
Fax: 631-632-8240
john.parise@sunysb.edu

RONALD E. STENKAMP (04)
Department of Biological Structure and Biomolecular Structure Center
University of Washington
Box 357420
Seattle, WA 98195–7420
Phone: 206-685-1721
Fax: 206-543-1524
stenkamp@u.washington.edu

CHERYL L. KLEIN STEVENS (05)
Department of Chemistry
Xavier University of Louisiana
1 Drexel Drive
New Orleans, LA 70125
Phone: 504-485-7377
Fax: 504-485-7942
cklein@xula.edu

ROBERT M. SWEET (03)
Biology Department
Brookhaven National Laboratory
Upton, NY 11973
Phone: 631-344-3401
Fax: 631-344-2741
sweet@BNL.GOV

IUCr Executive-President

BILL DUAX (05)
Hauptman-Woodward Med. Res. Inst.
73 High Street
Buffalo, NY 14203-1196
Phone: 716-856-9600
Fax: 716-852-4846
duax@hwi.buffalo.edu

Ex Officio Voting Members:

(see ACA roster for addresses)

RAYMOND E. DAVIS
ACA President

CHARLES CARTER
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ACA Treasurer

Subcommittee on Interdisciplinary Activities (non-voting members)

ALEX A. CHERNOV (03)
American Assoc. for Crystal Growth
Universities Space Research Assoc.
/AMMSA/NASA
Mail Code SD47, Bldg. 4481
George C. Marshall Space Flight Center,
Huntsville, AL 35812
Phone: 256-544-9196
Fax: 256-544-2102
alex.chernov@msfc.nasa.gov

JAMES A. KADUK (04)
ICDD Representative
(see USNCCr Officers for address)

JIAN-MIN (JAMES) ZUO (2005)
Microscopy Society of America
Materials Science and Engineering and
Materials Research Laboratory
Univ. of Illinois, Urbana-Champaign
1304 W Green Street, Urbana, IL 61801
Phone: 217-244-6504
FAX: 217-333-2736
jianzuo@uiuc.edu

Ex-Officio Non-Voting Members

Michael Clegg, (06)
NAS Foreign Secretary:
Dept of Botany and Plant Sciences
University of California, Riverside
1125 Batchelor Hall, Riverside, CA 92521
Phone: 909-787-4672
Fax: 909-787-4437
clegg@ucrac1.ucr.edu

ALICE P. GAST (6/30/03)
BCST Co-Chair
Stanford University*

WILLIAM KLEMPERER (6/30/04)
BCST Co-Chair
Harvard University*

Tamae Maeda Wong
NRC Program Director*

George York
NRC Senior Program Assistant*

***Send NRC/BCST correspondence to:**
DOUGLAS J. RABER
NRC/BCST Director
2101 Constitution Avenue, NW
Washington, DC 20418
Phone: 202-334-2156
Fax: 202-334-2154

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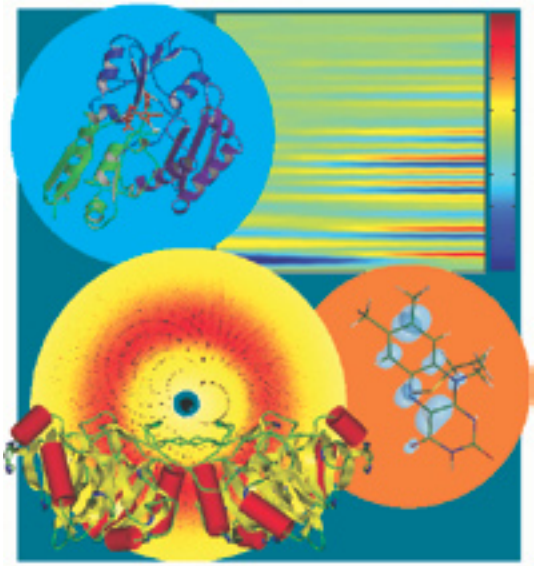


Upper left: from James Raftery and John Helliwell, University of Manchester, UK.: The ribbon diagram representation of the enzyme hydroxymethylbilane synthase in its active form determined by MAD at Daresbury SRS station 9.5. ***Determination of the structure of selenomethionine-labelled hydroxymethylbilane synthase in its active form by multi-wavelength anomalous dispersion,*** Hädener, A., Matzinger, P. K., Battersby, A. R., McSweeney, S., Thompson, A.W., Hammersley, A. P., Harrop, S. J., Cassetta, A., Deacon, A., Hunter, W. N., Nieh, Y. P., Raftery, J., Hunter, N. & Helliwell, J. R., *Acta Cryst* D55, 631-643, (1999). (This was published as the cover of that issue of *Acta D*.) This enzyme was also investigated by time-resolved Laue diffraction at ESRF ID09 as the crystal was fed substrate via a flow cell (Helliwell et al in *J Chem Soc Faraday Trans* 94(17), 2615-2622 and *J Chem Soc Faraday Discussions* (2002) vol 122).

Upper right: from Seol Ryu, Richard M. Stratt, and Peter M. Weber, Brown University, Providence, RI: **The image shows a calculated difference diffraction pattern of an 8-atom molecule, tetrazine, in the gas phase.** The scattering vector is plotted vertically, and the azimuthal angle about the electron beam is shown horizontally. Shown as contours are the differences between the diffraction pattern of the ground state, and the pattern upon laser-excitation of the S_1 electronic and the $16a^8$ vibrational state. This theoretical simulation suggest that the changes of the diffraction signal are on the order of 2%, which would make them experimentally observable. Experiments are underway to observe such vibrational diffraction patterns, and to explore their time dependence.

Lower right: from Roman Fedorov & Ilme Schlichting, Max Planck Institute, Dortmund, Germany: ***Crystal structures and molecular mechanism of a light induced signaling switch: the Phot-LOV1 domain from Chlamydomonas reinhardtii,*** R. Fedorov, I. Schlichting, E. Hartmann, T. Domratcheva, M. Fuhrmann and P. Hegemann. LOV (**L**ight **O**xygen **V**oltage) domains are the blue light sensors in the plant photoreceptor phototropin. Crystal structures of *Chlamydomonas reinhardtii* LOV1 in the dark resting state and of the covalent photoproduct intermediate occuring along the reaction cycle were determined to high resolution. They were used as a basis for quantum chemical calculations to deduce the mechanism of the photoreaction. The image shows the complex of the reactive Cys57 in its active conformation and the FMN chromophore. The highest occupied molecular orbital of the complex in the photoexcited triplet state is shown in blue. *Biophys. J.*, April/May 2003.

Lower left: from Andrew Mesecar, University of Illinois at Chicago: ***Laue x-ray diffraction pattern and structure of 2,4,5-Trihydroxytoluene Dioxygenase.*** This enzyme catalyzes a multi-step, multi-intermediate reaction whereby the aromatic ring of 2,4,5-trihydroxytoluene (a metabolite in the biodegradation pathway of the pollutant 2,4-dinitrotoluene), is cleaved. Each Laue image was produced from a 50 μs (10 pulses at 5 μs duration) exposure of x-rays generated at beamline 14-ID-B at BioCARS (Advanced Photon Source, Argonne National Laboratory). The final Laue structure of the enzyme was determined to 1.6 Å. Time-resolved Laue diffraction experiments are currently underway using photocaged substrates to initiate the reaction in the crystal with the hope that the intermediates of the reaction can be observed and identified.

ACA Communications Committee Update

The Communications Committee would like to keep the general membership updated on some of our activities and plans for the coming year, and most of all, to solicit your input. There are a number of areas where the Communications Committee can have a major impact on the ACA and the crystallographic community. Here are some of the things we are working on:

ACA email list - An up-to-date e-mail distribution list could be an invaluable asset when rapid communication among members is needed. However, as we found out with the BioMac SIG, the ACA e-mail list is sadly out of date, and many people did not get our correspondence. Maybe we should make it our goal to find a way to update this list.

ACA Web Site - The web site had a major facelift this past year. We would like it to become the primary source of rapid communication among our members. It allows us to inform the membership of changes to the meeting schedule, and other late breaking news, that the quarterly newsletter does not. At the same time, the ACA website should also provide a place for the SIGs and standing committees to have their own web pages, a starting point to help educators teach crystallography, and the primary source of communication with non-crystallographers. Our goal is to make the ACA web site the FIRST place one would look for any information about crystallography.

Crystallography Web Watch Column in the Newsletter - The Committee will continue to author this column in which web sites of particular interest to crystallographers are briefly summarized. The column has appeared in every newsletter since fall 2001. ACA members are urged to help in this effort by forwarding the addresses of favorite sites to the Committee chair.

Press Kit - We are interested in preparing a "press kit" for distribution to news media prior to our annual meeting. For example, for the upcoming meeting, we could prepare a press kit for distribution to the news organizations (TV, newspapers, etc.) in the greater Cincinnati area. Such a kit could contain both general information on the ACA and the impact of crystallography on science, and details on the upcoming annual meeting, including a copy of the program abstracts, etc.

Crystallography Books - The Committee is interested in keeping an on-line list of crystallographic books and publications, and finding ways we can make out-of-print books available to the crystallographic community.

Please feel free to contact us with any comments or suggestions that you might have. E-mail: **john.sack@bms.com**; telephone 609-252-5559, or fax 609-252-6030.

John Sack for the Communications Committee

ACA SUMMER COURSES

Small Molecule Crystallography

This course will be offered August 3 through 13, 2003 at the **Indiana University of Pennsylvania,** in the town of Indiana located about 80 miles east of Pittsburgh. There will be three 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 in 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 $294. Fifteen graduate student scholarships will be offered consisting of waivers of tuition and dormitory costs. Scholarships will be awarded based on the student's (1) scientific ability, (2) expected benefits from the course and (3) skills in English. Special funds will be available to assist applicants from Latin America.

Instruments available will be two Bruker-Nonius single crystal diffractometers (a CAD4 at IUP and a modern instrument with CCD detector located at the University of Pittsburgh and 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 Database and the ICDD Powder Diffraction Database.

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), **Patrick Woodward** (Ohio State Univ.) and **John Woolcock** (IUP).

The Course registration form can be obtained from the ACA web site at **http://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, or electronically by **Prof Charles 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 acknowledge sponsorship by the ACA, the IUCr, the Pittsburgh Diffraction Society and Bruker Axs, Inc. We 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

Macromolecular Crystallography

The **Illinois Inst. of Technology (IIT)** and the crystallographic community of the Chicago area will host an ACA-sponsored **Summer School in Crystallography** from Saturday, 12th July through Saturday, 26th July, 2003. The summer school will be conducted primarily on the campus of IIT, a small, well-respected technological university on the south side of Chicago, just across the expressway from Comiskey Park. We will take extensive advantage of the facilities of the Advanced Photon Source (APS) at Argonne National Laboratory; the APS is the brightest source of x-rays in the US, and it offers superb facilities for crystallography and other applications of x-rays.

Registration for the school will close around the end of May. Enrollment by non-local students will be limited to 40 students; we will also encourage local students to apply. We expect that the majority will be graduate students with some experience either in crystallography or a closely related field of chemistry or biochemistry, but we will accept postdocs and technicians. The registration materials are available on the ACA webpage.

The first eight days will be at IIT and at the other academic institutions in Chicagoland that have complementary laboratory facilities to IIT's. The remaining week of the school will be held partly at IIT and partly at the APS, where we have already received assurances of at least one day worth of beam time at six sectors; negotiations are underway for time at additional sectors. The faculty of the school is still being assembled, but we have confirmation of participation of the following crystallographers:

Andrew J. Howard, macromolecular crystallography; **Carlo Segre,** powder diffraction and EXAFS; **Thomas Irving,** fiber diffraction; **Timothy Morrison,** EXAFS; **Joseph Pluth,** chemical crystallography; **Edwin Westbrook,** macromolecular crystallography; **James Ibers,** chemical crystallography; **James Fait,** chemical & macromolecular crystallography; **Tristan Fiedler,** macromolecular crystallography.

Prof. Ibers is this year's recipient of the ACA's Buerger prize, and it is a particular honor to have him involved in the school. Non-local students will be staying in the dormitories at IIT, which are comfortable and readily accessible by public transportation from Chicago's airports. Bus transportation will be provided between IIT and the APS, and to special events. We plan social and scientific trips during the school, and will encourage students to travel directly from the school to the ACA's annual meeting in Cincinnati. The school ends the day the ACA meeting begins, and Cincinnati is a half-day's drive from Chicago, so the transition should be simple.

We welcome further inquiries from prospective students and faculty, and from companies that might wish to help sponsor the school. Nondiscrimination policies are identical to those of the *Small Molecule Course,* opposite. Please e-mail Andy Howard at **howard@iit.edu** for further information.

Andy Howard

Cele Abad-Zapatero in collage by Jeff Frye (Abbott) made from photos by R. Recacha. Translation of central panel: "*Sons, respectful and recognizing of Calvin, our great reformator, but condemning an error that was that of his century and firmly attached to the liberty of conscience, following the true principles of the Reformation and of Gospel, we have erected this expiatory monument on 27 October, 1903.*"

Notes of a Protein Crystallographer:

On the Shoulders of Giants

[The XIX Congress and General Assembly of the IUCr in Geneva]. . . was an excellent meeting full of lectures and symposia presenting and discussing new and exciting results. It was also a perfect venue to meet old friends from around the world in the civility and ambiance of an old European city and, in the evenings, to enjoy fondue at some of the restaurants near Cornavin train station or by the banks of the Rhône. Geneva is an amazing city.

. . . . The *vieille ville* has secluded cobble-stone streets that surround the imposing and austere protestant cathedral of St. Pierre from where the doctrines of Jean Calvin, the grand protestant reformator, influenced the course of European history. A few more turns up the hill, at 40 Grand Rue, one can find the birthplace of Jean Jacques Rousseau and a few doors down (at number 28) is the house that was the residence of the surrealist Argentinean writer José Luis Borges. Antique shops of all kinds –books, scientific instruments, crafts- and charming restaurants create a unique atmosphere.

The newer parts of the city also offer intriguing surprises, not unexpectedly connected to its illustrious and turbulent past. Next to the busy *Centre Médical Universitaire* there is an obscure street named after Michel Servet, a Spanish medical doctor who lived between 1511 and 1553. Coincidentally, on this street and precisely at No. 1, is the postal address and entrance to the world recognized Swiss-Prot Protein Knowledgebase, a resource that crystallographers and biomedical scientists consult constantly via the internet. Up a short slope in the avenue of Beau-Séjour and partly covered by vegetation, there is a simple stone slab erected on October 27, 1903 to commemorate the death of Michel Servet, burned at the stake at the nearby field of Champel on October 27, 1553. Beside the commemoration, the legend on the other side of the monument reads like a public and contrite apology for this infamous act. *(See figure legend.)*

What did Michel Servet do to deserve such horrendous agony? Who was Michel Servet? He was a very complex character who lived during the turbulent years of the protestant reformation in central Europe. . . [Servet studied original Greek and Hebrew versions of the Bible]. . . at the University of Toulouse, France. In 1531, at the early age of twenty, Servet published *De Trinitatis Erroribus* . . . attacking the orthodox teachings on the Doctrine of the Trinity for which he could not find any support in the Bible. His interpretations and complex speculations to explain the dogma of the Trinity in his own terms were clearly unacceptable to Protestants and Catholics alike . . . . Servet moved to Basel, Switzerland where the reception to his work was even more critical . . .[and he soon decided to leave] the hostile environment of Switzerland.

He moved to Lyon under the name of Villanovanus where he translated and published an excellent edition of *Ptolomy's Geography* in 1535. It was of such high quality and reputation that a second edition was produced in 1541. Between these publications, Servet tried to arrange for a meeting with John Calvin in Paris in 1534 to discuss his iconoclastic theological ideas. The meeting never took place, however, because Paris had already begun to prosecute heretics and Servet failed to arrive prior to Calvin's departure. These early events in Servet's life are witness to the scope of his interests and breadth of his knowledge as well the constant risks that he endured. . . .

[His friendship with the medical humanist Symphorien Champier] . . . led to Servet's authoring two incipient medical books. The first, *Leonardum Fuchsium Apologia* (1536) was just a defense of his friend against Leonhard Fuchs, but he managed to expound on his belief that certain herbs had healing powers. In 1537, he published what amounted to be a continuation of the *Apologia* entitled *Syruporum Universa Ratio*. This second medical treatise met with astounding success and went through six editions, allowing him to continue his studies of medicine in Paris. The work discussed in detail the curative virtues of certain syrups and contained passages discussing the use of citrus fruits as an aid in the digestion process. Both *Apologia* and *Syruporum* are considered to be significant contributions to modern pharmacologia.

. . . . Servet always lived as a devout Catholic but never abandoned his theological studies . . . His magnum opus is a unique theological treatise entitled *Christianismi Restitutio* that was published in 1553. Among other theological issues, he addressed the question of the introduction of the divine spirit into the blood and its dissemination throughout the body. Amazingly enough, it is within this context that Servet described for the first time to the Western world the discovery of the pulmonary circulation of the blood.

. . . Servet realized that there were clear inconsistencies between his observations of the circuitry of the blood vessels and the description proposed by Aristotle and Galen. He stated that the blood was not transmitted from the right ventricle of the heart to the left by way of a septum. Rather, given the size of the pulmonary artery, Servet concluded that blood passed through the lungs for oxygenation and subsequently the *"vital spirit is then*

transfused from the left ventricle of the heart into the arteries of the whole body." The ensuing discussion within *Christianismi Restitutio* suggests that he had reached essentially the complete explanation of circulation. The theological ruminations, however, make it difficult to know whether this was indeed the case. . . .It was not until 1694 that Servet's medical contribution was discovered and it is widely acknowledged that when Harvey announced his general scheme of blood circulation in 1628, he did not know of Servet's discovery.

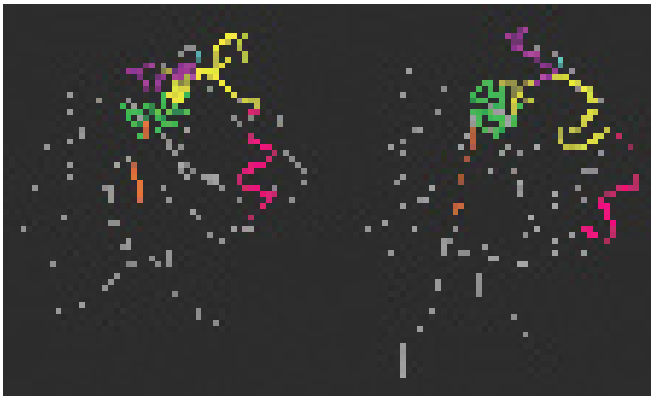
The publication of *Christianismi Restitutio* and the uncovering of the letters that he had written earlier to Calvin in Paris revealed the true identity of Michel de Villeneuve to the Lyon authorities and on April 4, 1553 he was arrested, expediently interrogated and imprisoned. Inexplicably, he managed to escape during the walk in the prison yard permitted to prisoners of his rank. . .. He remained in hiding in France for four months but decided to travel to Italy via Geneva. This decision proved to be fatal. He was recognized on August 13, speaking at the Church of the Madeleine and arrested. A long and thorough legal process followed resulting in Servet's sentence to be burned at the stake. ..Servet's last cry was a reaffirmation of his views on the Trinity.

As the saying goes, we rest on the shoulders of giants; on the shoulders of intellectual and ethical giants. . . . In the midst of our agonizing grant-writing periods, in the dark and gloomy days of grant renewal or even grant denial, we should remember that we are not risking our lives in order to pursue our intellectual curiosity. We are not vulnerable to imprisonment, torture and even death because we would like to understand certain biological processes. Our lives are not at stake because we explore daily the molecular intricacies of disease and pain. The results of our experiments are not life threatening. We do not risk imprisonment, trial and possibly death when our scientific ideas are printed. When our papers are rejected, we do not face torture or persecution; it just happens that our ideas are not of the main stream yet, or perhaps that our way of presenting them is not optimal. Some changes in the manuscript or additional experiments will solve the problem.

How many of us would continue to do what we are doing if our lives –not just our livelihoods- would be at risk? How many of us would get up in the morning and go to our well-equipped and expensive laboratories or synchrotrons if our scientific pursuits would put in jeopardy our very existence? These are very difficult questions to answer but it is important that we put our work and efforts in perspective . . . Our ability to follow our intellectual curiosity, and our extremely good fortune to make a living out of it, is currently possible because inquisitive people asserted their right to defend those ideals in the past. In our work, we depend on the labor and ethical pursuits of many others (past and present) for our inquisitive and intellectually satisfying professions as well as for our daily routines. Their efforts should be courteously appreciated and more importantly widely and profoundly acknowledged and recognized.

Cele Abad-Zapatero

Editor's note: Because of limited space, we were not able to publish Cele's article in full. However Cele has kindly promised to respond to email requests for his entire Servet biography including many notes, references and lengthy and sincere expressions of gratitude to Ms. Vivienne Baillie Gerritsen (Swiss-Prot Protein Knowledgebase). Write **cele.abad@abbott.com.**



D.Kern, B.Vokman, P.Luginbuhl, M.Nohaile, S.Kustu, D.Wemmer, (1999). Structure of a transiently phosphorylated switch in bacterial signal transduction. *Nature,* Vol 402, 894-898. and Vokman *et al* (1995) Three-Dimensional Solution Structure of the N-Terminal Receiver Domain of NTRC. *Biochemistry,* Vol 34, 1413-1324.

Quoting from David Marcey's website tutorial for this structure (© David Marcey, 2001): "The change of the position of a Mg^{++} would lead to an electrostatic repulsion between the phosphate group attached to the active site asp and the side chains . . . This repulsion . .(may cause) . . the backbone at arg56 to be released, enabling the rearrangement of the loop above the active site asp that connects beta strand 3 to alpha-helix 3."

Crystallography Web Watch

The ACA Communications Committee continues its "watch of the World Wide Web" 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.

Macromolecular museum — The Online Macromolecular Museum is a web site by David Marcey of California Lutheran University for the display of and information regarding macromolecular structures. Like any good museum, the "exhibits" are organized in "halls", in this case based on biological function. The structures exhibited range in complexity from the 20 amino acids to imunoglobulin and bacteriophage cro repressor. Each exhibit is tutorial in nature and allows interaction with the structure(s) being presented (e.g., rotation of molecules and switching between wire-frame and space-filling representations to illustrate structural details). A drawback is the requirement of Netscape 4.7.3 or less as a browser, with MDL Chime 2.0 or greater plug-in, to view and interact with the exhibits. However, these versions of both Netscape and the plug-in are still readily available for download and installation on your computer: **http://www.clunet.edu/BioDev/omm/gallery.htm**

Another Look: Reciprocal Net — (Reviewed in the Fall 2002 *Newsletter;* the address of this web site has changed since that review.) Reciprocal Net is a distributed database used by research crystallographers to store information about molecular structures. The project is a collaborative effort among Indiana University, Princeton University, the University of Cincinnati, the University of Minnesota, eight other universities, and the Los Alamos National Laboratory. Reciprocal Net also includes a nice teaching module on symmetry and point groups that is quite useful when incorporated in an advanced chemistry course: **http://www.reciprocalnet.org**

Books (and reviews) online — Looking for information on books of a crystallographic nature? Check out the Geometry.net web site **(http://geometry.net/basic_c_bk/crystallography_physics.html).** You also can find reviews of crystallographically related books on the British Crystallographic Association's **(http://bca.cryst.bbk.ac.uk/BCA/CNews/books/books.html)** as well as the IUCr's **(http://www.iucr.ac.uk/iucr-top/journals/bookreviews/)** web sites. And, for that out-of-print crystallography book, try **Bookfinder.com**, a search site from which some forty million titles, representing the collections of over 40,000 booksellers, can be viewed and purchased online via links to the booksellers **http://www.bookfinder.com**

Texture analysis — (Submitted by Virginia Pett.) A comprehensive course on the quantitative determination of crystallographic textures (a.k.a. preferred orientations) exhibited by materials from x-ray and neutron diffraction measurements is the subject of a web site by D. Chateigner and M. Morales. Lessons for the 11-session course are web based, and exercises and examinations are administered via electronic mail. Enrollment in the course requires tuition, and successfully completing the course nets a diploma for the happy student: **http://qta.ensicaen.ismra.fr**

Crystal Lattices — Many common crystal lattices and atomic packing schemes are described and depicted as crossed-stereo diagrams on Steven Watkins' web page made available by the Louisiana State University's Chemistry department **(http://www.chem.lsu.edu/htdocs/people/sfwatkins/ch4570/lattices/lattice.html).** The same material is also available on the MERLOT web site (see review in the Winter 2002 Newsletter), with the addition of 14 exercises and an answer key **(http://wb.chem.lsu.edu/htdocs/people/sfwatkins/MERLOT/flattice/00lattice.html)**. And, Brad De Gregorio has authored a handy web-based calculator for crystal plane d-spacings and angles between and zones specified by them and for zone axes and angles between them from known unit cell dimensions **(http://www.public.asu.edu/~bdegreg/Xtalplanes.html).** Input fields are provided for the Miller indices of up to six planes and three zone axes at a time.

Diffraction tutorials — An interactive tutorial on diffraction can be found on a web site by Thomas Proffen and R. B. Neder **(http://www.uni-wuerzburg.de/mineralogie/crystal/teaching/teaching.html).** The site provides a pictorial guide to atomic arrangements and their Fourier transforms, useful for teaching diffraction physics. Such diverse topics as powder diffraction, diffuse scattering and defect structures are covered. And for the macromolecular crystallographers in the crowd, the difference Patterson function is explained by example in a nice tutorial by Charles Brenner of Thomas Jefferson University's Kimmel Cancer Center **(http://asterix.jci.tju.edu/brenner/pr613.html)**

Crystallography Web Watch, con't

ICDD — (Submitted by Virginia Pett.): The International Centre for Diffraction Data (ICDD) is the place to find information and products related primarily to powder diffraction. It is home to the Powder Diffraction File, a database of some 300,000 experimental and calculated powder diffraction patterns from substances ranging from minerals and inorganic materials to organic compounds and pharmaceuticals. The ICDD holds tuition-based clinics on x-ray diffraction and x-ray fluorescence spectrometry, as well as international workshops in these areas, and sponsors the Denver X-ray Conference and the International X-ray Analysis Society's annual meeting. The organization also publishes the journal *Powder Diffraction*. For additional information, check out the ICDD web site: **http://www.icdd.com/**

Have a favorite web site that you'd like to see in a future **Crystallography Web Watch** column (and maybe linked on the ACA web site)? If so, send the web address and a short (1 or 2 sentence) description to **John Sack (john.sack@bms.com)**

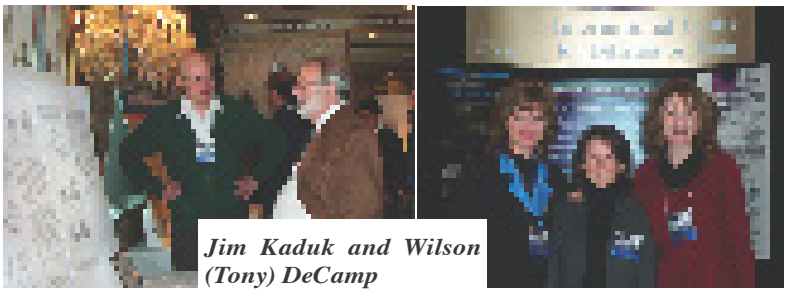
Pharmaceutical Powder X-ray Diffraction

2nd Symposium, December 9-12, 2002

The International Centre for Diffraction Data (ICDD) organized the 2nd Pharmaceutical Powder X-ray Diffraction Symposium, PPXRD-2. The Symposium was held in Concordville, Pennsylvania, on 9-12th December and had over 70 participants. The focus of the Symposium was on high-throughput crystallization and screening, polymorph characterization, and powder pattern indexing. The attendance was truly international with half the participants coming from 12 different countries.

A companion workshop, held on December 12th , 2002 focused on practical guides to powder pattern indexing and a discussion on round robins that can be used to help researchers compare their instrument performance with others in the pharmaceutical industry. There were 16 registrants for this hands-on workshop. The workshop focused on the steps in going from data collection through analysis to an indexed pattern. Examples and comparisons were made between conventional commercial x-ray equipment and synchrotron sources.

The first day was dedicated to acquisition and analysis of XRPD data. Creative approaches in pre-formulation and formulation were discussed. A comparative analysis between brand name drugs and generic drugs was given. Several presentations discussed the advantages of capillary sample holders, especially with single characteristic wavelength monochromators and parallel beam geometries. The second day focused on polymorph characterization. Results from challenging problems, including for example, determining the dynamics of dehydration in indapamide hemihydrate, using 'clustering' of low-quality XRPD patterns for phase identification, characterization of four polymorphs of fananserine, and high-throughput crystallization techniques that allowed up to ~300 crystallizations per day for a single lead compound were also clearly explained. The fananserine work showed the opportunity to connect structural results from x-ray powder diffraction with thermodynamic properties. Studies using structure determination techniques were discussed on a wide range of examples including zopiclone, anhydrous caffeine (Z'=5) and a compositionally disordered form of ranitidine HCl form 2. There were strong contributions from academia, pharmaceutical industry, analytical laboratories, equipment manufacturers and database organizations in all sessions.



Jim Kaduk and Wilson (Tony) DeCamp

PPXRD coordinators T.Maguire, L.Mooney and D.Raherty

The third day session on regulatory and patent issues focused on a number of well-known litigation cases including cefadroxil and ranitidine hydrochloride. The discussion focused on distinguishing differences between how courts interpret x-ray diffraction patents and how scientists interpret x-ray powder diffraction patterns. This session ended with several tutorial talks on SAXS and SANS. The focus was on contrast matching and other techniques to characterize length scale distributions up to several thousand Angstroms.

The fourth day Workshop featured lectures and a hands-on computer work (using WINPLOTR and FULLPROF) by Prof. Daniel Louër on indexing. Able assistance and lectures were provided by Jim Kaduk, Arnt Kern, Peter Varlaskin, and Fangling Needham.

The ICDD announced an exciting new relational database of organic materials targeted for pharmaceutical analyses. This product called PDF-4/Organics 2003 is immediately available containing 24,385 experimental entries and 122,816 calculated patterns. The database has more than 31 searchable fields, provides fully digitized powder patterns for both experimental and calculated patterns and contains integrated display software. This new database results from collaborations with the Cambridge Crystallographic Data Centre. Integrated data analysis packages utilizing the PDF-4/Organics database are available from several vendors.

I would like to acknowledge the excellent contributions and team effort from the PPXRD-2 Organizing Committee: Tomas Blanton, Harry G. Brittain, Noriaki Hirayama, Arnt Kern, Daniel Louër, Peter Munk, Fangling Needham, Richard Ortega, Peter Stephens, Gregory Stephens, Peter Varlashkin,

John Faber Chairman, Organizing Committee

The Inter-American Workshop on the Use of Synchrotron Radiation

Applications to Macromolecules and Biological Systems *December 09-11, 2002, LNLS, Campinas, Brazil*

The Inter-American Workshop on the use of Synchrotron Radiation (IAWS-2002) took place at the Campus of the National Synchrotron Light Source (LNLS) in Campinas, São Paulo, Brazil. This was the second Inter-American workshop organized in cooperation with the US Liason Committee to IUPAP (APS), and the (LNLS). These workshops are intended to be research-oriented and focused in specific areas of application of synchrotron radiation. The IAWS-2002 was dedicated to developments in Macromolecular and Biological Research. The main subjects were: crystallographic structure and function of proteins and biological systems, biopolymer assemblies and new polymer superstructures.

The three-day program was composed of 45 minute plenary lectures by invited speakers and poster presentations by the participants. The poster sessions had 42 contributions and took place in the afternoon of the second and third day of the meeting. Visits to the Laboratories of the campus were also organized for interested participants.

The topics included in the program were intended to cover a broad range of applications, all having in mind the potential use of the LNLS facilities (diffraction and spectroscopy synchrotron radiation beam lines of the 1.37 GeV electron ring as well as the NMR and Molecular Biology Laboratories). In the opening session José Antônio Brum presented a description of the LNLS facilities and the activities of its several research groups. This was followed by a presentation by Rogério Meneghini, giving an outline of the Structural Molecular Biology Program at the LNLS.

The lectures related to macromolecular structures and polymers dealt with recent advances in synchrotron radiation studies of polymer structures by Ben Chu, SUNY, the study of the controlled architecture of polymers in solution by Redouane Borsali from Bordeaux University, France, and the behavior of copolymer/surfactant complexes by Watson Loh from the University of Campinas, Brazil.

Marvin Hackert, from the University of Texas presented the first topic on protein folding: "Functional diversity from a simple protein fold". Sebastian Doniach (Stanford Linear Accelerator Center) described results from SAXS studies of "RNA folding and protein misfolding" which was followed by the very interesting work presented by Angel Garcia from Los Alamos National Laboratory on "All atom simulation of the folding/unfolding thermodynamics of small proteins and peptides". Very recent and outstanding theoretical results on this subject were brought by José Nelson Onuchic from the University of California, San Diego, dealing with all-atom calculations and minimalist models.

State of the art instrumentation and methods in synchrotron radiation applied to macromolecular structural studies were presented by William Shepard (European Synchrotron Radiation Facility) in an extremely didactic presentation of anomalous scattering methods and automation summarizing the fundamental concepts of the method and its optimized use. Robert Sweet (Brookhaven National Laboratory), talked about software, methods and training protocols to support mail-in and remote macromolecular crystallography at the NSLS. Igor Polikarpov (IFSC- USP) presented new technical developments at the LNLS and Ana Gonzalez (Stanford Linear Accelerator Center) completed the topic with a description of macromolecular crystallography data collection for high throughput projects.

On the subject of applications to drug design and disease-related macromolecules, Vivian Cody, from the Hauptmann-Woodward Medical Research Institute, brought us results on drug design strategies for AIDS-Pneumonia treatment. Jerson Lima (Universidade Federal de Rio de Janeiro) lectured on "Structure and dynamics of macromolecules involved in human diseases". Within this very important subject, a lecture on recent developments on drug design for parasitic diseases was presented by Glaucius Oliva (IFSC-USP, São Carlos) followed by novel results of the combination of spectroscopic and SAXS techniques used in the determination of the structural features of the human amyloid precursor protein, discussed by Sérgio T. Ferreira (Universidade Federal de Rio de Janeiro).

As a contribution to studies of biomolecules in solution and biomembranes, Sol Gruner (CHESS) described experiments on the effect of hydrostatic pressure on membrane lyotropes and proteins, illustrated with results of studies of myoglobin under pressure used to resolve the path of entry of the ligand to the heme binding site. Britt Thomas (Louisiana State University) presented his results on protein modulated phospholipid tubule self assembly and Vincent Licata (Louisiana State University) presented structural and functional properties of *T.aquaticus* and *E coli* DNA polymerases studied using various analytical techniques, which included SAXS measurements performed at LNLS.

With the purpose of giving a view of some important research programs going on at present in Brazil, three lectures were presented. The first one by Dario Grattapaglia (CENARGEN-EMBRAPA) on the recent developments of the project "Genoliptus: integrating genomics into Eucaliptus breeding for industrial forests" was extremely interesting showing an application of genomics with the aim of preserving natural forests. Wim Maurits Degrave (Fundação Osvaldo Cruz - FIOCRUZ) presented the important development of regional bioinformatics networks as integral part of genomics and proteomics in biotechnology, and the Latin American effort in this

respect with information on the *T cruzi* proteomics. Within the scope of applied research, César Chagas, from the Instituto Biológico de São Paulo described the use of transmission electron microscopy on viral morphogenesis and replication of plant viruses.

The incidental visit of Philip Bourne to Brazil during the period of this workshop gave us the opportunity of attending his presentation on the Protein Data Bank (PDB) and its relationship to the synchrotrons worldwide, aiming at the development of a comprehensive data resource that will contain the structures and all stages of the experiments involved in their determination.

The number of participants reached 114, which was more than we expected, given the short time we had for the organization of this workshop. This number includes the lecturers and organizers. The lecturers whose participation was funded by APS were: Benjamin Chu, Angel Garcia, Robert Sweet, Sol Gruner, Ana Gonzalez, Sebastian Doniach and José Nelson Onuchic. One graduate student, Alexei Suarez Soares, was also sponsored by APS.

The participation of two other lectures (Britt Thomas and Vincent Licata) as well as Paul Russo and two graduate students from Louisiana State University, Allison M. Joubert and Greg Thomson) was funded by the NSF/LSU-IGERT program.

The roll of 10 lecturers whose participation was funded by the Laboratório Nacional de Luz Síncrotron (LNLS) and other Brazilian Agencies (FAPESP) includes Marvin Hackert (USA), Vivian Cody (USA), William Shepard (ESRF, France), Redouane Borsali (France), Dario Grattapaglia (Brazil), César Chagas (Brazil), Wim Maurits Degrave (Brazil), Sérgio T. Ferreira (Brazil), Igor Polikarpov (Brazil), Glaucius Oliva (Brazil), Jerson Lima (Brazil).

Eight participants from Latin American countries were granted travel funds provided by the Latin American Center for Physics (CLAF) and the Brazilian National Research Council (CNPq – PROSUL program); other expenses were funded by LNLS. The recipients of these grants were: Marcelo Rubio (Argentina), Silvia Cuffini (Argentina), Daniel Roberto Vega (Argentina), Daniel Fernández (Argentina), Pedro Hernandez (Chile), Silvia Russi Uruguay), Gabriela Servilia Jimenez (Venezuela), Cristian Carlos Puig (Venezuela).

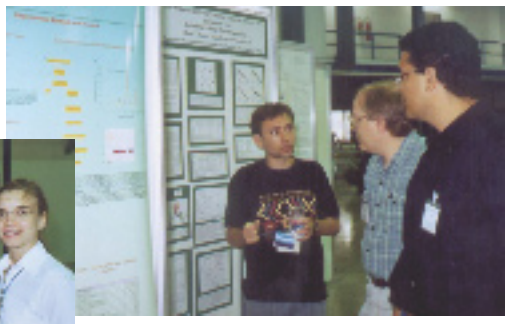
In order to make participation possible, it was decided to grant a waiver of the registration fee to Brazilian and Latin American graduate students. Most of them could not have afforded this payment. The lecturers and senior participants were lodged in a Campinas center city hotel. The LNLS Guest House offered lodging for the rest of the participants. The LNLS also provided transportation to/from the Hotel to the Campus, and lunches at the cafeteria.

Iris L. Torriani, Chair, IAWS Organizing Committee

José Antônio Brum at the opening session

Gabriela Servilia Jimenez (Venezuela); Pedro Hernández (Chile); Silvia Russi (Uruguay); Daniel Fernandez (Argentina); Daniel Veja (Argentina); Silvia Cuffini (Argentina); Cristian Carlos Puig (Venezuela)

Bob Sweet, (Brookhaven National Laboratory), presenting his lecture



Tomás Plivelic (LNLS); Paul Russo (LSU) and Cristiano L.P. Oliveira (Unicamp)

Visiting the SAXS beamline: Ben Chu (SUNY); Iris Torriani (LNLS); Britt Thomas (LSU); Marvin Hackert (Univ. of Texas)

Seb Doniach (SLAC); Wm. Shepard (ESRF); Sol Gruner (CHESS); Beatriz Guimaraes (LNLS)

Rosalind Franklin: The Dark Lady of DNA by Brenda Maddox, HarperCollins, New York, 2001, ISBN 0-06-018407-8

Reviewed by Eugenie V. Mielczarek

In 1951, the race to publish the structure of DNA was heating up with the fanaticism apropos of an athletic contest. That race ended in 1953, when Rosalind Franklin's unpublished measurements of the crucial distances in the DNA molecule were provided without her knowledge to James Watson and Francis Crick, enabling them to build a model of DNA. Many scientists think Franklin deserved to share the Nobel Prize awarded to Watson, Crick, and Maurice Wilkins in 1962 for determining the structure of DNA. She had died four years earlier at the age of 37, and the prize is never awarded posthumously.

Brenda Maddox's ***Rosalind Franklin: The Dark Lady of DNA*** is a meticulous study of a brilliant scientist and a chronology of an epochal scientific adventure. Maddox is a science journalist, an editor for the *Economist*. No details of Franklin's personal or scientific life escaped her. Maddox interviewed scientists, talked with Franklin's relatives, and read her personal and scientific correspondence. Maddox is a prize-winning biographer; Franklin was a perfectionist. The biographer and her subject are well matched.

My introduction to Rosalind Franklin was through reading James Watson's *The Double Helix* (Atheneum, 1968). Watson's now infamous personal descriptions of her are a well-remembered chapter in scientific history. It is difficult to read any biography of Franklin dispassionately. The first biography of Franklin, *Rosalind Franklin and DNA* (W. W. Norton, 1975), was by her personal friend Anne Sayre. Maddox did not know Franklin, and wrote with a 44-year perspective. The success of Maddox's biography is that its extensive scholarly detail eases the reader into objectivity.

Maddox devotes four chapters to Franklin's childhood and formal education. From her family life, Franklin learned to trust her judgments, live modestly, and scorn self-indulgence. She understood her capabilities and was forthright about speaking up, an unexpected and perhaps unwelcome trait for a female scientist.

At the age of 21, Franklin started her research on crystalline materials in support of an important wartime project. Coal was used in gas masks during World War II, and Franklin investigated why some kinds of coal are more impervious than other kinds to gas and water. Because of her expertise on "holes in coal," in 1947 Jacques Mehring invited her to join the Laboratoire Central des Services Chimiques de l'Etat in Paris. In Mehring's lab, she latched onto x-ray crystallography and used it to study disordered carbon crystals. In chapters 5 and 6, Maddox describes Franklin in Paris as "a woman of the Left Bank"--happy, beautiful, successful, and valued by colleagues.

Franklin's success landed her at King's College, London, in 1951, with a fellowship to study proteins in solution and in dehydrated forms. Before leaving Paris, she carefully designed the apparatus she would need. Her major concern was to control the humidity and temperature of the samples. When she arrived at King's College, the focus of the project changed from protein solutions to biological fibers, particularly DNA. Control of humidity was a serious issue, because DNA fibers lengthen as they hydrate, and the motion blurs the photographs. Franklin was already familiar with such problems through her work with crystalline forms of coal.

Although scientifically fortuitous, the move to King's College carried the seeds of dissent. The lab director, John Turton Randall, informed Franklin by letter that only she, Ray Gosling (a graduate student), and an assistant would be working on her project. However, Randall was already studying DNA fibers with Maurice Wilkins. Randall and Wilkins needed Franklin's x-ray diffraction experience, but offered her only a three-year fellowship, with neither rank nor academic appointment. Understandably, the laboratory relations between Franklin and Wilkins were uncomfortable.

In nearby Cambridge, investigators at the Cavendish laboratory were also using x-ray diffraction to examine complex biological molecules. Also at Cambridge was Francis Crick, a PhD student, who was joined by James Watson in 1951. Watson and Crick undertook to find the structure of DNA by model building. Naturally, they needed measurements of DNA's crystalline parameters, but lacked the experimental technique and resources. In *Genes, Girls, and Gamow: After the Double Helix* (Knopf, 2002, p. 8), Watson explains: "I hoped to expand the attention of the unit to DNA . . . once I had learned x-ray diffraction techniques." Adding to that hurdle, Lawrence Bragg, head of the laboratory, told Watson and Crick to cease work on DNA because British scientific politics gave priority to Randall's group.

Meanwhile, Franklin labored intensely in a hostile atmosphere. (Even Watson, on p. 20 of *The Double Helix*, admitted that at King's, "the best home for a feminist was in another person's lab.") Her x-ray photographs and laborious calculations "suggested a helical structure . . . with the phosphate groups on the outside." She discovered the B (wet) form of DNA, and was the first to photograph it and to measure the spacing between the bases and the cylindrical repeat distance. She wanted to delay her final decision about the structure until she and Gosling were completely convinced by the data. However, without her or Gosling's knowledge, Wilkins showed Watson and Crick the crucial x-ray photograph of the B form and gave them the crystalline parameters she had laboriously calculated. The 25th April, 1953 issue of *Nature* carried three papers on the subject: by Watson and Crick; by Wilkins, Alec Stokes, and Herbert Wilson; and by Franklin and Gosling.

Franklin continued her scientific career at Birkbeck College, where she tackled the structure of the tobacco mosaic virus, a subject more challenging than DNA. In his 1982 Nobel lecture, Aaron Klug--her closest collaborator and friend--acknowledged her contribution to his own work on molecular structure.

Maddox brings out one fact not generally known: *The Double Helix* was originally scheduled to be published by Harvard University Press. The outcry from eminent scientists and from Franklin's family was so intense that Harvard's board of overseers asked the press to drop the book. Atheneum later published it.

Maddox's mastery of historical detail gives us a definitive portrait of this warm and brilliant scientist and represents the science in an accurate and approachable way.

Reprinted from *Physics Today,* Feb., 2003, p. 61. ©2003, American Institute of Physics. Eugenie V. Mielczarek is emeritus professor of physics at George Mason University. She has worked in materials science and biological physics and is coauthor of *Iron, Nature's Universal Element,* Rutgers U. Press, 2000. **(Ed. note: See Letters to Editor, page 4.)**

Introduction to Macromolecular Crystallography

by Alexander McPherson. John Wiley & Sons; (October 2002) ISBN: 0-47-125122-4

Reviewed by Helen M. Berman

The first crystal structure of a protein was reported a little over forty years ago when John Kendrew announced the structure of myoglobin. Determination of the structure of hemoglobin by Max Perutz followed closely thereafter. Thus began the golden era of protein crystallography that is now responsible for more than 15,000 macromolecular structures.

The early pioneers in the field were firmly grounded in physics. Indeed, without this understanding it would not have been possible to collect the data let alone interpret its meaning. I entered the field of X-ray crystallography as protein structures were first beginning to appear. My training involved reading texts by Buerger and James, and long homework assignments that included exercises such as deriving the structure factor expressions for various space groups. Everything took a long time, and so there was time to learn.

As x-ray crystallography has given way to structural biology, and as technology has made it possible to determine structures in months, then days, and now hours, crystallographic training has changed. For the most part, training continues to be done as an apprenticeship in a research laboratory. Fundamental knowledge is often gained from textbooks that usually focus on very practical aspects of the field. One outstanding example is the book on crystal growth *(Crystallization of Biological Macromolecules)* by Alexander McPherson. If a university department has a resident crystallographer, a course may be given and sometimes the course contains the fundamental underpinnings of the discipline. Often the elements of crystallography are relegated to a few lectures in a survey course in biophysics or biochemistry.

For the last fifteen years, the Cold Spring Harbor Laboratory has sponsored a short and intense course in macromolecular crystallography where students learn how to do crystal structure analysis. This course has been well received and there are many well-known graduates, some of whom have made seminal contributions to structural biology. As part of the course, students receive didactic training in the theoretical aspects of the field. Those lectures, given informally by Alexander McPherson, have now been collected in a volume entitled *"Introduction to Macromolecular Crystallography"*.

This book is excellent. McPherson explains some very complex and even philosophical concepts in a straightforward way. At first he uses amusing language to tackle difficult questions. For example, he asks, "What is a structure?" and gives some sample answers including a quotation from the song "The Purple People Eater". He then goes on to discuss how one would be able to understand and discover the structure of a Volkswagen Beetle using first basketballs, tennis balls and ping-pong balls as probes. Having captured our attention, McPherson then goes on to the serious business of describing the properties of crystals, waves, and diffraction. Each chapter builds on information presented in the previous ones; the reader is thus constantly reminded of the basic concepts. The book is relatively short and with the exception of refinement, very few of the essential points are missed.

Alex McPherson

As every teacher of crystallography knows, it can be very difficult to decide at what level to present the concepts that underlie the discipline. Indeed it can be tempting for some teachers to avoid dealing with some of these concepts since so much of crystallography is automated. This practice is dangerous and could potentially results in creating a generation of scientists who would not be able to tackle the real challenges in structural biology such as macromolecular assemblies or membrane proteins.

I recommend this book very highly to anyone who is teaching a course in crystallography and certainly for biologists wanting to grasp the basics of the field.

Reprinted from: *Biochemistry and Molecular Biology Education* (Article 0188) Eds: voet@sas.upenn.edu jvoet1@swarthmore.edu

Crystallization Technology Handbook, Alfons Mersmann, Ed., 2nd Edition, (2001) Marcel Dekker, Inc., New York – Basel, ISBN: 0-82-470528-9

Reviewed by Alex Chernov

This big volume consists of 15 chapters of which 10 (~500 pages) are written by A. Mersmann and his co-workers: 1. Practical and Chemical Properties of Crystalline Systems, 2. Activated Nucleation, 3. Crystal Growth, 4. Particle Size Distribution, 5. Attrition and Attrition Controlled Secondary Nucleation, 6. Agglomeration, 7. Quality of Crystalline Products, 8. Design of Crystallizers, 9. Operation of Crystallizers, 10. Challenges in the Overview of the Control of Crystallizers, 11. Reaction Crystallization, 12. Tailor-Made Additives and Impurities, 13. Suspension Crystallization from the Melt, 14. Layer Crystallization and Melt Solidification, 15. Thermal Analysis and Economics of Processes. The Appendix (41 pages) provides solubilities, heats of crystallization and some kinetic information for 173 inorganic and organic systems organized in tables and is a valuable asset to the text.

The book is for industrial engineers and is written mainly by industrial engineers. It's scope spans a vast area of industrial crystallization, predominantly from solutions (13 of 15 chapters). These crystallization processes result in polycrystalline powder, agglomerates or layers (the latter in the purification processes by melt crystallization). The processes include primary and secondary nucleation of crystals in solution or seeding, interfacial crystal growth phenomena, mass and heat transfer, various kinds of mixing, collisions of the crystallites with the crystallization tank walls, mixing propellers and with other crystallites. Product quality, including its size distribution function, is based on chains of these interrelated processes.

All these components are addressed in different chapters. Broad scope, simple approach and straightforward style certainly make the book attractive for practitioners. Presentation of each subject includes a general qualitative description and attempts to quantitatively characterize processes and products. The authors' inclination to characterize phenomena quantitatively should be appreciated.

However, this is not easy because of the complexity and multi-parametric nature of the processes. The equations and graphs used in the book are numerous, especially in the first part of the book, and are usually on the easy-to-follow algebraic and empirical level, employed in the design of crystallizers and to describe their operation. The quantities and parameters involved are listed in "Notation" expanded over 11 pages. Unfortunately, the parameters required are not always available in the literature and thus in the book. For instance, there are only a few examples of kinetic coefficients characterizing rates of various growth processes. This, however, is partly compensated by Table A1.3 in the Appendix providing references to some of the original publications where nucleation and/or growth kinetics have been measured for salts in aqueous solutions. There is no extensive discussion or tables for distribution coefficients of impurities, inclusion trapping, and other purification issues of primary importance for industrial crystallization. On the other hand, qualitative description of the "taylor made impurities" present the state of the art.

In general, the book covers major problems and includes updated useful information for those engineers and researchers who deal with industrial crystallization.

Intimate Triangle: Architecture of Crystals, Frank Lloyd Wright and the Froebel Kindergarten by Jeanne Spielman Rubin, Polycrystal Book Service, Huntsville AL, 2003, **http://www.polycbs.com** ISBN 0-97-187760-2

The "*Intimate Triangle*" is a narrative about the lives and works of three men whose disciplines are closely interwoven: Frank Lloyd Wright, the architect, Christian Samuel Weiss, a crystallographer, and Friedrich Froebel, an educator. The principles of shapes and lines introduced in the Froebel kindergarten have produced the basis for many of Wright's designs in architecture. Christian Samuel Weiss was regarded by many as the father of the science of crystallography. This book explores his relationship with Friedrich Froebel, father of the "Froebel kindergarten" to which Frank Lloyd Wright attributed much of his success. *From Polycrystal book release*.

Crystal Growth Technology by K. Byrappa & T. Ohachi (eds.), William Andrew Publishing, (December 2002), ISBN 0-81-551453-0

This book deals with almost all the modern crystal growth techniques that have been adopted, and includes appropriate case studies. The book begins with "Growth Histories of Mineral Crystals" by a senior expert in this field, Professor Ichiro Sunagawa. The next chapter reviews recent developments in the theory of crystal growth. The book then moves on to techniques: 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 the publisher's web site:* **http://www.williamandrew.com/titles/1453.html**

A Century of Physics by D. Allan Bromley, Springer-Verlag, New York, (2002), ISBN 038-795247-0.

D. Allan Bromley used the occasion of the centenary of the American Physical Society to reflect upon the growth of physics over the past 100 years, its fragmentation into numerous subdisciplines, the impact physics has had upon modern technology, and the re-emergence of the fundamental unity of the discipline in recent years. Hundreds of historical illustrations accompany the text. Bromley conveys much of the excitement and wonder that research in physics generated in the 20th century and asks what new things are in store in the next century. He covers such topics as relativity and quantum mechanics, the Manhattan project, superconductivity, transistors and the revolution brought about by solid-state electronics, protein folding, the uses of nuclear and atomic physics in biology and medicine, plate tectonics, the expansion of the universe and the Big Bang, and gravitational radiation. Bromley is Sterling Professor of the Sciences and Dean of Yale University. *From the publisher's web site*.

Ivory Bridges: Connecting Science and Society by G. Sonnert. MIT Press, Cambridge, MA (2002). ISBN 0-262-19471-6

The examination of science policy is guided by the notion of *"Jeffersonian science"*-defined as basic research on topics identified as being in the national interest. The book illustrates the concept with a case study of the Press-Carter Initiative of the late 1970s and proposes that a Jeffersonian approach would make a valuable addition to future science policy. Citizen-scientists who have organized themselves to promote the welfare of society are also discussed. An extensive appendix profiles many of these organizations. *Courtesy of Amazon.com. All rights reserved; www.amazon.com.*

Our Cosmic Habitat by Martin Rees. Princeton U. Press, Princeton, NJ (2001) ISBN 0-691-08925-4

"In this book, Martin Rees, one of the leading figures in theoretical astrophysics, offers the reader his unique perspective on the field and introduces many of the most exciting new results and ideas in astronomy." *(David N. Spergel, Princeton University; from back cover of paperback edition.)* Martin Rees is Royal Society Research Professor at Cambridge University, Astronomer Royal of Great Britain and author, most recently, of the bestselling *Just Six Numbers: The Deep Forces That Shape the Universe*.

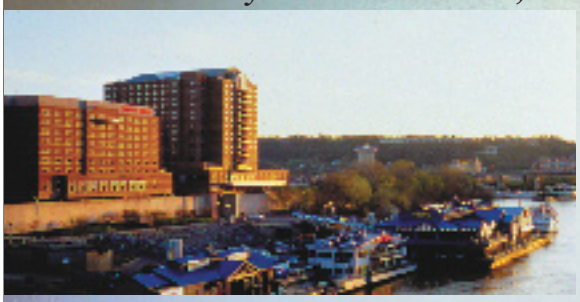
The Golden Ratio, The Story of Phi, the World's Most Astonishing Number by Mario Livio. Broadway Books; (2002) ISBN: 076-790815-5.

Euler's constant, Ø, the ratio obtained "*when the whole line is to the greater segment as is the greater segment to the lesser*" (also the ratio of the diagonal of a regular pentagon to the side), is the irrational number with value approximately 1.618 associated with Fibonacci numbers and natural growth patterns. Phi has fascinated mathematicians and scientists since geometry began, and deserves to have its story told. Mario Livio heads the Science Division at the Hubble Space Telescope Institute.

International Tables for Crystallography: Volume E: Subperiodic Groups, V. Kopsky and D.B. Litvin, eds. This new volume in the series covers the seven frieze groups, the 75 rod groups and the 80 layer groups. For more information please visit **http://www.iucr.org/iucr-top/it/index.html**

ACA 2003, July 26-31, 2003

Northern Kentucky Convention Center, Covington, KY



The organizers of ACA2003 invite you to attend an action-packed week of science and fun!

Covington, Kentucky is located across the Ohio River from Cincinnati, Ohio and is minutes from the Cincinnati/Northern Kentucky International Airport. All scientific sessions, posters and the exhibit show will be held in the Northern Kentucky Convention Center **(http://www.nkycc.com/)**.

The ACA2003 meeting (http://www.che.uc.edu/aca/) agenda:
Workshops: **Saturday, July 26**
Scientific Symposia and Sessions: **Sunday, July 27- Thursday, July 31**
Poster Sessions: **Sunday, July 27-Tuesday, July 29**
Vendor Exhibits & Sponsored Activities **scheduled throughout the week**
Consult the Call for Papers for detailed information on workshops and sessions

Social Events:
Saturday, July 26—Opening Reception: *Newport Aquarium*
Sunday, July 27—Mentor/Mentee Dinner: *Chez Nora*
Monday, July 28—Midweek Mixer: *Jack Quinn's Irish Pub*
Wednesday, July 30—Banquet: *Embassy Suites Hotel*
Thursday, July 31—Riverboat Dinner Cruise

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

Symposia:
Transactions Symposium: **Neutron Diffraction** (co-organizers: Gerry Bunick & Leif Hanson)
Special Symposium: **Time-Resolved Crystallography** (co-organizers: Phillip Coppens & Keith Moffat)
Martin J. Buerger Award Symposium: **2003 Awardee** is **Dr. James Ibers** (Northwestern U.)
Bertram Warren Award Symposium: **2003 Awardee** is **Dr. Takeshi Egami** (U. Pennsylvania)

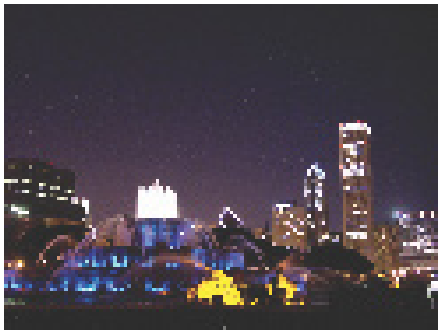
Important Upcoming Dates:
Advanced Registration deadline: June 1, 2003
Advanced Hotel Registration deadline: June 24, 2003

On-line registration and further meeting information will be posted to the ACA2003 site at **http://www.che.uc.edu/aca/** or see the ACA web site: **http//www.hwi.buffalo.edu/ACA/**

Local Chair: Bobby Barnett, U. Cincinnati, **barnettbl@cinci.rr.com**
Program Chair: Jeanette Krause Bauer, U. Cincinnati, **jeanette.krause@uc.edu**
Social Chair: Ann Wolff, Procter & Gamble, **wolff.am@pg.com**

ACA 2004
July 17-22—Chicago, IL

The annual meeting of the ACA will be held in downtown Chicago at the Hyatt Regency Hotel on Wacker Drive. The hotel is located on the Chicago Riverwalk along the south side bank of the Chicago River adjacent to Michigan Avenue, nicknamed the "Magnificent Mile," and near Lake Michigan, Lake Shore Drive, and Grant Park. The conference and exhibition will be held in the East Tower of the hotel. The banquet will be in the Crystal Ballroom in the West Tower of the hotel, overlooking the Tribune and Wrigley buildings. Navy Pier, the Art Institute, the Field Museum, Shedd Aquarium, Adler Planetarium, and the Museum of Contemporary Art are all located nearby. Grant Park is the site for several summer festivals and concerts. Both airports, O'Hare and Midway, are located within twenty miles of the downtown area.



Chicago is home to several universities, and is a city of great restaurants, jazz and blues venues, museums, theaters, sport's teams, etc. Here are some websites that might be interesting to explore:

chicagoreader.com . . . .Great for restaurant listings, concert listings, etc.
jazzinstituteofchicago.org . . .Information on jazz clubs, concerts, etc.
chicago.il.org . . . Good tourism site, and check out the free trolley system.
cityofchicago.org . . . Good tourism site, and help in getting around town.

Photos of Chicago are courtesy of Terry and Melody Howe, ChicagoPhotography.com.

Visa Alert from *FASEB News*, February, 2003

We have heard reports indicating that some foreign scientists are having difficulty getting their visas processed in time to assure attendance at scientific meetings. As part of new security procedures, many visa applications are being sent to the State Department in Washington, DC for review by a variety of federal agencies. Due to the number of visas being processed and the heightened security concerns, this review can take as long as six to eight weeks, or longer, depending on the applicant's country of origin.

We encourage U.S. scientists going overseas to check with their respective university for resources relating to travel and visa issues abroad EARLY IN THE PLANNING PROCESS, in the event of reciprocal delays. We also encourage scientists intending to come to the United States to apply for visas AS EARLY AS POSSIBLE and to pay attention to U.S. State Department guidance on this matter.

The National Academies has a very useful website containing information about this situation. See **http://national-academies.org/visas.** The most frequent reason that visitor visas are denied is that the applicant failed to provide enough evidence, in the opinion of the consular officer, that there was no intention to immigrate to the United States. Therefore, we encourage you to pay particular attention to State Department advice on how to deal with this type of denial. For more information, see **http://travel.state.gov/visadenials.html.**

PROGRAM CHAIRS:
Christer Aakeröy: aakeroy@ksu.edu
Marilyn D. Yoder: myoder@cctr.umkc.edu

LOCAL CHAIRS:
Bernie Santarsiero: bds@uic.edu
Karl Volz: kvolz@uic.edu;

Meeting Calendar

MAY 2003

12-17 **Charge Density Workshop** at the Chemistry Department, SUNY, Buffalo. **http://harker.chem.buffalo.edu/group/announcement/xd.html**

19-21 **2003 NSLS Users' Meeting,** Upton, NY, **http://nslsweb.nsls.bnl.gov/nsls/users/meeting/**

JUNE 2003

ICDD 2003 X-ray Diffraction Clinics: website: **http://www.icdd.com/**

2-6 **Fundamentals of X-ray Powder Diffraction**

9-13 **Advanced Methods in X-ray Powder Diffraction**

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

17-21 **Relantenz: Latin American Workshop on Enzyme Technology**, Varadero Beach, Matanzas, Cuba. Contact: Reynaldo Villalonga, Univ. of Matanzas, **relatenz.umcc@umcc.cu, relatenzworkshop@yahoo.com.** Website: **http://www.umcc.cu/relatenz/**

22-27 **Gordon Conference: Proteins**, Holderness School, Plymouth, NH, , Chairs: Rachel E Klevit & Lynne J Regan. **http://www.grc.uri.edu/programs/2003/proteins.htm**

JULY 2003

12-26 **ACA Summer School in Macromolecular Crystallography**, Illinois Inst. of Technology, Chicago, IL. Contact Andrew Howard, **howard@iit.edu**

13-18 **Gordon Conference: X-ray Physics**, Roger Williams U., Bristol, RI. Doon Gibbs, Chair. Website: **http://www.grc.uri.edu/programs/2003/xray.htm**

20-24 **International Congress of Biochemistry and Molecular Biology,** Toronto, CA. **www.iubmb2003.org**

21-26 **Aperiodic-2003,** Belo Horizonte, Brazil. **http://agora.grude.ufmg.br/aperiodic2003**

26-31 **American Crystallographic Association Annual Meeting, ACA 2003,** Covington, KY. **Local Chair: Bobby Barnett, barnettbl@cinci.rr.com; Program Chair: Jeanette Krause Bauer, jeanette.krause@uc.edu** **(see p. 38)**

AUGUST 2003

3-13 **ACA Summer Course in Small Molecule Crystallography,** Indiana University of Pennsylvania, **Bryan Craven, craven@icubed.com; Charles Lake, lake@grove.iup.edu.** **(see p. 23)**

10-13 **AsCA'03/Crystal-23,** Cable Beach Club resort, Broome, Western Australia. **http://www.broome2003.uwa.edu.au/**

14-15 **Biological StructureWorkshop,** Cable Beach Club resort, Broome, Western Australia. (website above)

14-19 **Sagamore Meeting** (IUCr Commission on Charge, Spin and Momentum Densities), Cable Beach Club resort, Broome, Western Australia. (see website above).

24-30 **21st European Crystallographic Meeting,** Durban, South Africa , **http://www.ecm21-africa.co.za/**

SEPTEMBER 2003

2-6 **ECNS 2003 European Conference on Neutron Scattering,** Montpellier, France. Contact: R. Vacher, **rene@ldv.univ-montp2.fr**

3-7 **5th International Conference On Molecular Structural Biology (ICMSB2003),** Vienna, Austria. Conference Secretariat: Dr. Andreas Kungl, Austrian Chemical Society (GÖCH), **andreas.kungl@kfunigraz.ac.at**

14-19 **Structure Solution from Powder Diffraction Data, SSPD'03;** Congress Center Academia, Stara Lesna, Slovakia. **http://www.sspd-03.sav.sk**

OCTOBER 2003

6-10 **Introduction & Advanced X-Ray Diffraction For Pharmaceutical Applications,** Danbury, CT

JUNE 2004

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

JULY 2004

17-22 **American Crystallographic Association Annual Meeting, ACA 2004,** Chicago, IL. **Chairs: Bernie Santarsiero, bds@uic.edu; Karl Volz, kvolz@uic.edu; Christer Aakeröy, aakeroy@ksu.edu; Marilyn Yoder, myoder@cctr .umkc.edu** **(see p. 39)**

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/**

Postdoctoral position: Macromolecular

SUNY at Buffalo / Hauptman Woodward Medical Research Inst. Position available for macromolecular crystallographer. Must have experience in protein expression and purification; experience with construction of mutants is desirable; to work in Program in Proteomic and Genomic analysis of the short chain oxido reductase family of enzymes, especially members of the family linked to hypertension, cancer, Alzheimer's and polycystic kidney diseases. A new Ph.D.preferred with possibility of three years of support. The candidate would be encouraged to develop an independent project during the second and third year. Please send c.v. and three letters of reference to: Dr. William L. Duax, Dept. of Structural Biology SUNY at Buffalo, Hauptman Woodward Medical Research Inst., 73 High St., Buffalo, NY 14203.