

**SAN ANTONIO** May 25-30 2002  
*Transactions Symposium  
on Powder Diffraction*

*Table of Contents*

President's Column .....1-2  
 Council News .....3  
 On the Cover.....5  
 2002 ACA Officers, Appointments .....7  
 2002 ACA Roster of Committee & SIG Officers .....8-11  
 FYI: Congressional Calendar.....11  
 USNCCr Roster, 2002 .....13  
 Max Perutz.....14  
 Deane K. Smith.....15  
 Don C. Wiley .....16-17  
 ACA Corporate Members .....17  
 WebWatch .....19  
 Bionet Crystallography note .....19  
 SBC Call for Synchrotron Beamline Proposals .....21  
 Deadline Extended for Summer School Proposals .....25  
 Ira Flatow to Receive Wood Award .....25  
 Ira Flatow's Book List.....27-32  
 ACA '02 Contributors and Exhibitors .....32  
 San Antonio ACA Meeting .....33-35  
 Workshop on Non-Merohedral Twinning .....37  
 Meetings and Workshops .....37  
 Calendar of Meetings and Schools .....39  
 Contributors to This Issue.....39  
 Positions Available.....40

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

<i>...Connie Chidester</i>	<i>Judith L. Flippen-Anderson</i>
<i>...2115 Glenwood Dr.</i>	<i>Code 6030</i>
<i>...Kalamazoo, MI 49008</i>	<i>Naval Research Laboratory</i>
<i>...</i>	<i>Washington, DC 20375</i>
<i>...tel. 616-342-1600</i>	<i>tel. 202-767-3463</i>
<i>...fax 716-852-4846</i>	<i>fax 202-767-6874</i>
<i>...conniechidester@earthlink.net</i>	<i>flippen@nrl.navy.mil</i>

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  
 E-mail [marcia@hwi.buffalo.edu](mailto:marcia@hwi.buffalo.edu)

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

ACA Newsletter (ISSN 1958-9945) Number 1, 2002. 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*



I'd like to begin this, my inaugural message to the ACA, with an expression of gratitude, on behalf of the ACA Council, to all the volunteers who contribute their valuable time to make this organization work, especially the Local and Program Chairs of meetings, our SIG and Standing Committee officers, and our intrepid *Newsletter* Editors.

One is often free to rejoice in the influx of new and younger members. This issue, we balance that response by mourning the loss of Max Perutz, Don Wiley, and Deane Smith. The macromolecular community, in particular, will always retain the joy of Max's far-reaching scientific and personal contributions and the lasting contributions of Don's intellect and incisive style. The 1971 Cold Spring Harbor meeting, where I met both for the first time, is surely a crystalline moment in time, so resonant is Wayne Hendrickson's sensitive recollection with my own. Don's T-shirt remains every bit as profound an icon for me as it is for Wayne. There is nothing that assures us of success in what we do; we profit gratefully from the lives and lasting gifts of all three men, and our profound sympathy goes out to their family and friends.

This year's annual meeting in San Antonio is a Spring meeting, because the IUCr Congress and General Assembly will be held later this summer in Geneva. Meeting planning generally attempts to locate the triennial spring meeting in an extra-specially inviting venue, and from what I experienced at last year's Council meeting in San Antonio, they succeeded wildly. San Antonio will provide the attendees with an absolutely unique environment designed for fun and fellowship. The rivercenter development offers a rich variety of restaurants and bars for eating and socializing, and is a splendid place to walk or to run. It is long and interesting enough to engage even the more aggressive runners, and it presents a different face for each time period during the day. An almost entirely different atmosphere surrounds the Convention Center above ground, which sits not far from the Alamo and within shouting distance of many other historic landmarks, including the platform from which Teddy Roosevelt recruited many of the "Rough Riders"! The Local Chairs, Marv Hackert and Ray Davis, (who is also our new Vice President), have done a bang-up job securing the best facilities and planning a series of festive opportunities to renew friendships and learn details of the latest developments they've heard about during the scientific program itself.

Speaking of the program itself, Wally Cordes and Travis Gallagher have put together a program with an unusual number of novelties, some of which signal potential new directions for the ACA. The work of this year's Patterson Award winner, Doug Dorset, has inspired symposia on

Electron Crystallography organized by Bill Duax (two half-days), and on Electron Microscopy of Biological Macromolecules organized by Bob Glaeser (four half-days). A host of newcomers to the ACA meetings will gather for these symposia, and we hope that some of them, or perhaps most, will find it worth their while to stay on as members.

A fond hope for many years at both the ACA and the USNCCr has been to promote more meaningful participation in Society affairs by crystallographers from Latin and South American countries. Last year, the IUCr reinforced these desires in their message to the US National Committee. As a result, the ACA Council decided on a plan to enable greater participation from this region in the San Antonio meeting. These guests will participate in all phases of the program. Our goal is to move toward a situation similar to that of the Canadian crystallographers, in which membership and participation in ACA affairs is normalized and the community is represented on the ACA Council. We will address the question of how to strengthen this effort and solve the associated problems during Council meetings in San Antonio. I welcome your input into this initiative, and, especially, I urge all of you to make an extra effort to engage these guests while at the meeting.

Charlie Carter

### **International Centre for Diffraction Data® Ludo Frevel Crystallography Scholarships**

#### **Recipients of the 2002 Scholarships are:**

**Dane A. Boysen**, of Caltech, Pasadena, California with research involving “*Hydrogen-Bonding, Phase Transitions, and Proton Conductivity in  $MH_2PO_4$ -Type Solid Acids ( $M=Li, K, Na, Rb, Cs$  and  $NH_4$ )*”

**Desiree H. Fong**, of McGill University of Montreal, Quebec, Canada with exploration into “*Structural Analysis of an Antibiotic-Detoxifying Kinase*”

**Jeffrey H. Haeni**, of Pennsylvania State University, University Park, Pennsylvania with major interest in “*Growth and Characterization of Metastable  $BaTiO_3/SrTiO_3$  Superlattices*”

**Michael W. Lufaso**, of Ohio State University, Columbus, Ohio with studies on “*Evaluation and Prediction of the Crystal Structures of Single/Ordered/Disordered Octahedral Cation Perovskites Using the Software Program SPuDS*”

**Jeffrey P. Maranchi**, of Carnegie Mellon University, Pittsburgh, Pennsylvania with research concerning “*Novel Chemical Synthesis and Characterization of Electrode Materials for Thin Film Lithium-Ion Batteries*”

**Christine M. Clark McCracken**, of the University of Manitoba, Winnipeg, Manitoba, Canada who's investigating “*The Crystallography and Chemistry of Tourmaline*.”

The ICDD will present each of these students with \$2,250 to help them continue their studies in their selected fields of crystallographic research.

### **John Helliwell Named CCLRC's Director of Synchrotron Radiation Science**

John Helliwell, Professor of Structural Chemistry at the University of Manchester, one of the founding editors of the *Journal of Synchrotron Radiation* and the Editor-in-Chief of *Acta Crystallographica*, became the Council for the Central Laboratory of the Research Councils' Director of Synchrotron Radiation Science based at Daresbury Laboratory on a five-year secondment from the University. John Helliwell has had close links with the laboratory since 1979. The post involves all the operational and scientific matters regarding the operation and development of the Synchrotron Radiation Source, as well as involving corporate responsibilities for advising CCLRC on its strategic direction in the field of synchrotron radiation.

from *J. Synchrotron Radiation* **9**, 47, (2002)

### **New APS Beamlines for Structural Biology**

The National Institute of General Medical Sciences (NIGMS) and the National Cancer Institute (NCI) are supporting the design and construction of a user facility consisting of three new beamlines at Argonne National Laboratory's Advanced Photon Source. The beamlines themselves will be custom designed and constructed by ACCEL GmbH, a company located in Bergish Gladbach, Germany. NIGMS and NCI plan to spend a total of around \$23 million on the project and estimate that the three beamlines will be fully operational in about three years.

“The primary motive for the project is to benefit the scientific community by facilitating access to synchrotron beamlines. This is particularly important as the structural genomics effort at NIGMS begins to pick up speed,” said Dr. Marvin Cassman, Director of NIGMS.

NCI is particularly interested in how the synchrotron facilities will advance the study of cancer-related molecules. “A detailed understanding of protein structure will help cancer researchers develop drugs targeted to specific types of cancer,” said Dr Dinah Singer, Director of NCI's Division of Cancer Biology.

from *J. Synchrotron Radiation* **9**, 47, (2002)

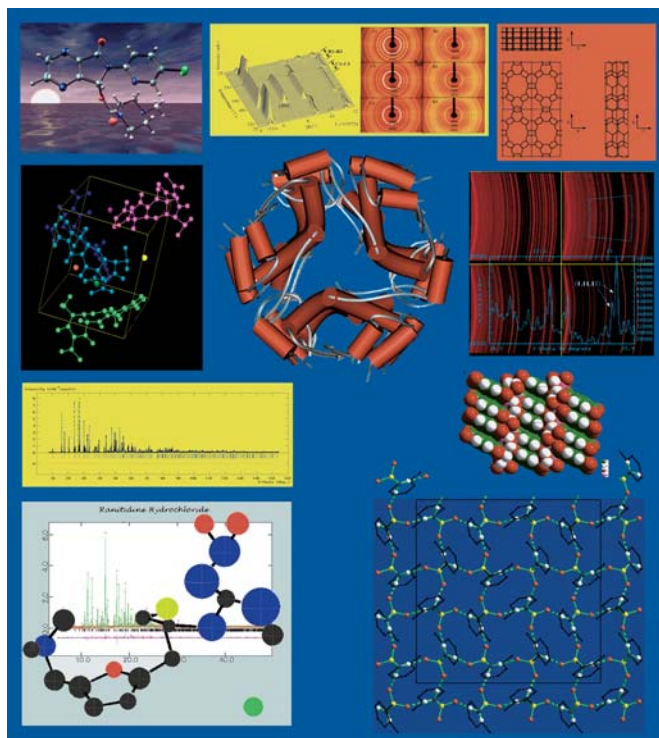
### **Wade Adams Now CNST Director at Rice**

*Houston, Feb. 14, 2002* – Wade Adams, former chief scientist at the Air Force Research Lab (AFRL), at Wright-Patterson Air Force Base in Dayton, Ohio, became the new director of the Center for Nanoscale Science and Technology (CNST) at Rice University in January.

Adams has B.S. and M.S. degrees in physics from the U.S. Air Force Academy, and Vanderbilt University, and a Ph.D. in polymer science and engineering from the University of Massachusetts. He worked for 32 years at the Wright-Patterson Air Force Base, where he was responsible for providing consultative and advisory service to the AFRL until his retirement Jan. 3rd. He is a fellow of the American Physical Society and of the Air Force Research Laboratory. His research in polymer physics has concentrated on structure-property relations in high-performance organic materials, high-performance rigid-rod polymer fibers, X-ray scattering of fibers and liquid crystalline films, polymer-dispersed liquid crystals and theoretical studies of polymer properties.

Office of Media Relations, Rice University

On the Cover: Images from the Transactions Symposium



Center:

**From Robert Von Dreele:** an “end view” of the TRDC Zn-insulin complex. The structure was “solved” from powder diffraction data taken at NSLS beamline X3B1 (*Acta Cryst. D*, December, 2000). One TR block is rotated 15 degrees with respect to the next one down the c-axis. The c-axis is therefore doubled.

Clockwise from upper left:

**From William I.F. David:** metastable zopiclone. (Zopiclone is the active ingredient in some sleeping tablets – hence the setting sun.) Thermodynamic evidence indicates that the structure transforms from one stable polymorph, a racemic monoclinic dihydrate to another non-centrosymmetric orthorhombic anhydrous form through a metastable intermediate polymorph. Using high-temperature *in-situ* synchrotron X-ray powder diffraction, we were able to isolate and subsequently determine the crystal structure of this intermediate anhydrous monoclinic phase and to provide a clear explanation for the dehydration mechanism in zopiclone. (N.Shankland, W.I.F.David, K.Shankland, A.R.Kennedy, C.S.Frampton, A.J.Florence, *Chem. Comm.* **21**, 2204-5 (2001).)

**From John Parise:** time-resolved *in situ* synchrotron X-ray powder diffraction patterns were taken at NSLS beamline X7 on Pb-rho, heated and cooled under atmosphere. Details of the phase transition are shown as series of frames from the IP detector (right). (“*Understanding negative thermal expansion behavior and “trap-door” cation relocation in zeolite rho*” B.A.Reisner, Y.Lee, J.Hanson, G.Jones, J.B.Parise, D.A.Corbin, B.H.Toby, A. Freitag, J.Larese, and V.J.Khalenberg, *Chem. Soc., Chem. Comm.*, **22** 2221-2222, (2000).)

**From Michael Deem:** SSZ55, recently solved in collaboration with Stacey Zones. (“*Synthesis and Structure Determination by ZEFSAII of SSZ-55: A New High-Silica, Large-Pore Zeolite,*” M.G.Wu, M.W.Deem, S.A.Elomari, R.C.Medrud, S.I.Zones, T.Maesen, C.Kibby, C.-Y.Chen, and I.Y.Chan, *J. Phys. Chem. B* **106** 264-270 (2002).)

**From John Parise:** selected images taken on a Bruker Smart 1000 CCD at the NSLS X7A synchrotron X-ray powder diffraction beamline as a function of time during the 6 h of K-exchange into Na-Low silica Zeolite X(LSX). The 1-D patterns are obtained by integrating the CCD data. These data can be used for Rietveld structure refinement and allow resolution of the atomistic mechanism responsible for the phase change as K replaces Na in the zeolite. (Y.Lee, C.Cahill, J.Hanson, J.B.Parise, S.Carr, M.L.Myrick, U.V.Preckwinkel, and J.C.Phillips, *Proceedings of the 12th International Zeolite Association Meeting*, Baltimore, Maryland, July 5-10 1998, *Materials Research Society (Vol I-IV)*, M.M.J.Treacy, B.K.Marcus, M.E.Bisher & J.B.Higgins (Eds), Vol. IV 2401 – 2408 (1999).)

**From Jim Kaduk:** image from a paper recently submitted to *Acta Cryst. B*: “*Terephthalate salts of dipositive cations*”, J.A.Kaduk. The paper describes a set of four isostructural compounds (Mg, Mn, Fe, and Co) solved using synchrotron data taken at NSLS beamline X3B1 and lab powder data. Quantum calculations were carried out on all four structures to locate the hydrogens and understand the hydrogen bonding.

**From Maryjane Tremayne:** the crystal structure of 2-toluenesulfonamide CHCHSONH; one of a number of arenesulfonamides solved from laboratory X-ray powder diffraction data using the direct-space based differential evolution technique. The molecules are linked by two N-HO=S hydrogen bonds forming spiral chains (C(4)) and sixteen-membered rings (R(16)). These motifs combine to form a secondary hydrogen bond network illustrated by projection of the structure on the (001) plane, showing the R(16) and R(12) rings linking the C(4) chains into an elegant three-dimensional framework. Christopher Glidewell, School of Chemistry, University of St Andrews, UK, collaborated in this work.

**From Peter Stephens:** The background is a Rietveld refinement of data we took at NSLS beamline X3B1 on Ranitidine HCl (Zantac®). The molecule is almost the correct structure, determined *ab initio* from powder data. Ranitidine turns out to have a conformational disorder, and if you don’t know that when you solve the structure, you get the absurd thermal parameters shown. The message is that simulated annealing solutions of powder structures are sufficiently sophisticated that poor results tell you that the starting model was wrong. (The picture as well as most of the work in the solution was done by Peter’s student, Ashfia Huq.)

**From Hideo Toraya:** The diagram is a fitting result of Rietveld refinement for alpha-SiN, which is a typical ceramic material. (H. Toraya, *J. Appl. Cryst.* **33**, 95-102 (2000).)

**On the Cover, con't**

**From Armel Le Bail and Lachlan M.D. Cranswick:** Structure plot of the antibiotic tetracycline hydrochloride, solved by Armel Le Bail from laboratory powder X-ray diffraction data and refined using the FULLPROF Rietveld software. Data from this sample was used in the 1998 Structure Determination by Powder Diffractometry Round Robin organized by Armel Le Bail and Lachlan M.D. Cranswick. The image was rendered using GRETEP for Windows (Jean Laugier and Bernard Bochu) and POV-Ray, Persistence of Vision<sup>(TM)</sup> (Ray Tracer).

**ACA COUNCIL OFFICERS - 2002**

**PRESIDENT**

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

**VICE PRESIDENT**

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

**PAST PRESIDENT**

**William C. Stallings**  
 Pharmacia  
 700 Chesterfield Village Pkwy  
 Chesterfield, MO 63198  
 (636) 737-7236  
 Fax: (636) 737-7425  
 william.c.stallings@pharmacia.com

**TREASURER**

**Douglas Ohlendorf**  
 Dept. of Biochem., Mol. Biol. & Biophys.  
 6-155 Jackson Hall  
 Univ. of Minnesota  
 Minneapolis, MN 55455  
 (612) 624-8436  
 Fax (612) 624-5121  
 ohlen@dcdiff.med.umn.edu

**SECRETARY**

**Lee Brammer**  
 Dept. of Chemistry  
 Univ. of Sheffield  
 Sheffield S3 7HF  
 UK  
 44 144 222 9536  
 lee.brammer@sheffield.ac.uk

**CANADIAN REPRESENTATIVE**

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

**CANADIAN DIVISION**

**Gary Enright, Chair(01-02)**  
 Steacie Inst. For Mol. Sciences  
 NRC 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

**IUCr REPRESENTATIVE / EXECUTIVE OFFICER**

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

**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

**APPOINTMENTS**

**FINANCIAL OFFICER**

**S.N. Rao, Dean**  
 College of Grad. Studies & Res.  
 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

**NEWSLETTER EDITORS**

**Judith Flippen-Anderson**  
 Code 6030  
 Naval Research Laboratories  
 Washington, DC 20375  
 (202) 767-3463  
 Fax: (202) 767-6874  
 flippen@nrl.navy.mil

**Connie Chidester**  
 2115 Glenwood Dr.  
 Kalamazoo, MI 49008  
 (616) 342-1600  
 conniechidester@earthlink.net

## STANDING COMMITTEES 2002

### COMMUNICATIONS

**Frank Rotella (02)**

Biological Div, Bldg 202  
Argonne National Laboratory  
9700 S. Cass Ave.  
Argonne, IL 60439-4833  
Tel: (630) 252-3830  
Fax: (630) 252-6126  
fjrotella@anl.gov

**Jack 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 Krause Bauer (04)**

Dept. of Chemistry  
University of Cincinnati  
P.O. Box 210172  
Cincinnati, OH 45221-0172  
Tel: (513) 556-9226  
Fax: (513) 556-9239  
jeanette.krause@uc.edu

**Kay Onan (05)**

Northeastern University  
100 Meserve  
Boston, MA 02115  
Tel: (617) 373-2102  
Fax: (617) 373-5015  
k.onan@nunet.edu

### DATA, STANDARDS & COMPUTING

**Victor G. Young (02)**

Dept. of Chemistry  
University of Minnesota  
207 Pleasant Street SE  
Minneapolis, MN 55455  
Tel: (612) 625-6897  
Fax: (612) 626-7541  
young@xray1.chem.umn.edu

**John Huffman (03)**

Dept. of Chemistry  
Indiana University  
Bloomington, IN 47405  
Tel: (812) 855-6742  
Fax: (812) 855-8300  
huffman@indiana.edu

**Helen Berman (04)**

Chem/Wright & Rieman Labs  
Rutgers University  
610 Taylor Road  
Piscataway, NJ 08855  
Tel: (732) 445-4667  
Fax: (732) 445-4320  
berman@rcsb.rutgers.edu

**Jeffrey R. Deschamps (05)**

Naval Research Lab  
4555 Overlook Avenue SE  
Washington, DC 20375  
Tel: (202) 767-0656  
Fax: (202) 767-6874  
deschamps@nrl.navy.mil

### CONTINUING EDUCATION

**Bryan Craven (02)**

Dept. of Chemistry  
Indiana Univ of Pennsylvania  
Indiana, PA 15705  
Tel: (412) 357-5784  
craven@grove.iup.edu

**Winnie Wong-Ng (03)**

Materials Sci & Eng. Div.  
Bldg. 223 Room A256, NIST  
Gaithersburg, MD 20899  
Tel: (301) 975-5791  
Fax: (301) 975-5334  
winnie.wong-ng@nist.gov

**Philip Fanwick (04)**

Dept. of Chemistry  
Brown Laboratory  
Purdue University  
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  
University of California Davis  
One Shields Avenue  
Davis, CA 95616  
Tel: (530) 752-6668  
Fax: (530) 752-8995  
olmstead@indigo.ucdavis.edu

## SPECIAL INTEREST GROUP OFFICERS 2002

### *Biological Macromolecules*

**Celerino Abad-Zapatero - Chair**

Protein Crystallography Lab D-46y, 100  
Abbott Park Rd  
Bldg. 10 AP-10 L-07  
Abbott Park, IL 60064-6098  
Tel: (847) 937-0294  
Fax: (847) 937-2625  
cele.abad@abbott.com

**Vivian C. Yee – Chair-elect**

Molecular Cardiology/NB20  
Cleveland Clinic Avenue  
9500 Euclid Foundation  
Cleveland, OH 44195  
Tel: (212) 444-2057  
Fax: (212) 445-1466  
yeev@ccf.org

**Alice Vrieling – Sec./Treas. (03)**

Dept of Biology  
Univ. of California Santa Cruz  
Sinsheimer Labs 1156 High St  
Santa Cruz, CA 95064  
Tel: (831) 459-3929  
Fax: (831) 459-3139  
vrieling@biology.ucsc.edu

## Fiber Diffraction

### Thomas C. Irving – Chair

Bio Chemical and Physical Science  
 Illinois Institute of Technology  
 3101 Dearborn  
 Chicago, IL 60616  
 Tel: (312) 567-3489  
 Fax: (312) 567-3494  
 irving@biocat1.iit.edu

### Jennifer Taylor – Sec./Treas.(03)

Dept. of Materials Science  
 University of Cambridge  
 Pembroke St.  
 Cambridge CB2 3Q7, UK  
 Tel: 44 1223 762 866  
 Fax: 44 1223 334 567  
 jet50@cam.ac.uk

## General Interest

### Gloria E Borgstahl - Chair

Dept of Chem/Wolfe Hall 3214  
 Univ. of Toledo  
 2801 W. Bancroft St.  
 Toledo, OH 43606-3390  
 Tel: (419) 530-1501  
 Fax: (419) 530-4033  
 gborgst@uoft02.utoledo.edu

### Hugo Steinfink – Chair-elect

Dept of Chem. Engineering  
 University of Texas Austin  
 Austin, TX 78712  
 Tel: (512) 471-5233  
 Fax: (512) 471-7060  
 steinfink@che.utexas.edu

### Vivian Cody – Sec./Treas. (03)

Hauptman Woodward MRI  
 73 High Street  
 Buffalo, NY 14203-1196  
 Tel: (716) 856-9600 ext. 322  
 Fax: (716) 852-6086  
 cody@hwi.buffalo.edu

### Judy Flippen-Anderson - Member at Large (02)

Code 6030  
 Naval Research Laboratories  
 Washington, DC 20375  
 Tel: (202) 767-3463  
 Fax: (202) 767-6874  
 flippen@nrl.navy.mil

## Materials Science

### Scott T. Misture - Chair

NYS College of Ceramics  
 Alfred Univ.  
 Two Pine St., Alfred, NY 14802  
 Tel: (607) 871-2438  
 Fax: (607) 871-2392  
 misture@alfred.edu

### Charlotte Lowe-Ma – Chair Elect

Physics Department  
 MD 3028 SRL  
 Ford Research Lab  
 Dearborn, MI 48121  
 Tel: (313) 317-7382  
 Fax: (313) 322-7044  
 clowema@ford.com

### Richard Harlow – Sec./Treas.(02)

7 Shull Drive Devon  
 Newark, DE 19711  
 Tel: (302) 695-2097  
 Fax: (302) 695-1351  
 rharlow@conective.net

### Douglas A. Keszler – Member at Large (02)

Dept. of Chemistry  
 Oregon State University  
 Corvallis, OR 97331-4003  
 Tel: (503) 737-6736  
 Fax: (503) 737-2072  
 keszlerd@ccmail.orst.edu

## Neutron Scattering

### Simon J Billinge - Chair

Dept. of Physics & Astronomy  
 Michigan State Univ.  
 East Lansing, MI 48824  
 Tel: (517) 353-8697  
 Fax: (517) 353-4500  
 billinge@pa.msu.edu

### Thomas Proffen – Chair Elect

Los Alamos National Laboratory  
 Manuel Lujan Dr. Neutron Scattering  
 Center  
 LANSCE-12, MS H805  
 Los Alamos, NM 87545  
 Tel: (505) 665-6573  
 Fax: (505) 665-2676  
 tproffen@lanl.gov

### James Richardson – Sec./Treas. (03)

IPNS Div.  
 Argonne National Lab  
 9700 S. Cass Avenue  
 Argonne, IL 60439  
 Tel: (630) 252-3554  
 Fax: (630) 252-4163  
 jwrichardson@anl.gov

## Service Crystallography

### Paul Boyle - Chair

Dept of Chemistry  
 North Carolina State Univ.  
 Box 8204, Raleigh, NC 27695  
 Tel: (919) 515-7362  
 Fax: (919) 515-5079  
 boyle@chemdept.chem.ncsu.edu

### Richard Staples – Chair-elect

Dept of Chemistry  
 Harvard University  
 12 Oxford Street 237  
 Cambridge, MA 02138  
 Tel: (617) 495-0787  
 Fax: (617) 496-5618  
 staples@chemistry.harvard.edu

### Michael Carducci - Sec/Treas (02)

Dept. of Chemistry  
 University of Arizona  
 Tucson, AZ 857-0041  
 Tel: (520) 621-4168  
 Fax: (520) 621-8407  
 carducci@u.arizona.edu

## Small Angle Scattering

### Paul Butler – Chair

Bldg 7962 Stop 6393 (Room 214)  
 Oak Ridge Nat'l Lab  
 PO Box 2008  
 1 Bethel Valley Rd.  
 Oak Ridge, TN 37831-6393  
 Tel: (865) 576-6067  
 Fax: (865) 574-6268  
 pcb@ornl.gov

### Jinkui Zhao – Chair-elect

Spallation Neutron Source  
 Oak Ridge National Lab  
 701 Scarboro Road  
 Oak Ridge, TN 37830-6474  
 Tel: (865) 574-0411  
 Fax: (865) 241-5177  
 zhaoj@ornl.gov

**Pete Jemian – Sec./Treas. (03)**

UNICAT, Bldg. 438D  
 Advanced Photon Source  
 Argonne National Laboratory  
 9700 South Cass Avenue  
 Argonne, IL 60439  
 Tel: (630) 252-0863  
 Fax: (630) 252-0862  
 jemian@anl.gov

**Peggy Cebe Member at Large (02)**

Dept. of Physics & Astronomy  
 Science & Technology Center Rm  
 208, Tufts University  
 4 Colby St., Medford MA 02155  
 Tel: (617) 627-3365  
 Fax: (617) 627-3744  
 peggy.cebe@tufts.edu

**Synchrotron Radiation**
**James F. Fait – Chair**

SER-CAT  
 34 Kentland Drive  
 Romeoville, IL 60446  
 Tel: (630) 252 0644  
 Fax: (630) 252-0641  
 fait@anl.gov

**Young Scientists**
**Nicholas Silvaggi - Chair**

Dept. of Mol & Cell Biology  
 Univ. of Connecticut  
 75 N Eagleville Rd  
 Storrs, CT 06269  
 Tel: (860) 486-2099  
 Fax: (860) 486-2099  
 nrs98001@uconnvm.uconn.edu

**C. Kent Brown – Chair Elect**

Dept. of Biochemistry  
 University of Minnesota  
 Church Street  
 Minneapolis, MN 55455  
 Tel: (612) 625-5175  
 brow0927@te.umn.edu

**Johanna Mazlo – Sec./Tres. (02)**

Dept. of Chemistry  
 Univ. of Nebraska at Lincoln  
 750 Hamilton Hall Box 750  
 Lincoln, NE 68588-0304  
 Tel: (402) 472-8894  
 Fax: (402) 472-0168  
 jmazlo@uninfo.unl.edu

**Small Molecules**
**John C Bollinger - Chair**

Dept of Chemistry  
 Indiana Univ.  
 Bloomington, IN 47405  
 Tel: (812) 855-5560  
 Fax: (812) 855-8300  
 jobollin@indiana.edu

**Brian Patrick Chair-elect**

Dept. of Chemistry  
 University of British Columbia  
 2036 Main Mall  
 Vancouver, BC V6T 1Z1  
 Tel: (604) 822-4865  
 brian@xray5.chem.ubs.ca

**Joseph Reibenspies – Sec./Treas. (03)**

Dept. of Chemistry  
 Texas A&M Univ.  
 College Station, TX 77843-3255  
 Tel: (409) 845-9125  
 Fax: (409) 845-8184  
 reibenspies@mail.chem.tamu.edu

**American Institute of Physics FYI: Congressional Calendar**

On February 4, President Bush submitted his FY 2003 budget request to Congress, starting the appropriations cycle for fiscal year 2003, which begins on October 1, 2002. Below is the tentative congressional calendar for the remainder of the year. Because it is an election year, Members of Congress will try to spend as much time as possible in their state or district offices, and will try to wrap up their work early enough to campaign before the elections in November. However, with Members trying to stake out positions prior to the election, and with a projected deficit looming, this is likely to be a difficult and contentious session. Visiting with your Members of Congress can be one of the most effective ways of communicating your views. This year, you may be more likely to find them available if you set up a visit at their local state or district offices, particularly during one of the House's District Work Periods. Please see "Communicating with Congress" on the AIP web site [www.aip.org/gov](http://www.aip.org/gov) for more information on planning an effective visit with your Members of Congress.

**CONGRESSIONAL CALENDAR FOR 2002:**

May 27 - 31	Memorial Day District Work Period
July 1 - 5	Independence Day District Work Period
July 26	Summer Recess Begins - House
August 2	Summer Recess Begins - Senate
September 3	Return from Summer Recess
September 16	Congress Not In Session - Yom Kippur
October 4	Targeted Adjournment Date
November 5	General Elections



**USNCCr Officers**

**Marvin Hackert, Chair (02)**

Dept. of Chem. and Biochem.  
University of Texas at Austin  
Austin, TX 78712  
Phone: 512-471-1105  
Fax: 512-471-8696  
m.hackert@mail.utexas.edu

**Jon Clardy, Vice-Chair (02)**

Dept. of Chem. & Chem. Biol.  
Cornell University  
Ithaca, NY 14853-1301  
Phone: 607-255-7583  
Fax: 607-255-1253  
jcc12@cornell.edu

**Winnie Wong-Ng,**

Secy/Treas(02)  
Ceramics Division, NIST  
Bldg. 223 Room 256  
Gaithersburg, MD 20899  
Phone: 301-975-5791  
Fax: 301-975-5334  
winnie.wong-ng@nist.gov

**Members**

**Lonny E. Berman (02)**

Nat'l Synchrotron Light Source  
Brookhaven Nat'l Laboratory  
Bldg. 725D, P.O. Box 5000  
Upton, NY 11973  
Phone: 631-344-5333  
Fax: 631-344-3238  
berman@bnl.gov

**Joel D. Brock (04)**

Appl. and Eng. Physics  
Cornell University  
210A Clark Hall of Science  
Ithaca, NY 14853-2501  
Phone: 607-255-0639  
Fax: 607-255-7658  
jdb20@cornell.edu

**Subcommittee On  
Interdisciplinary Activities  
(non-voting members)**

**Alex A. Chernov, Rep., AACG**

Universities Space Res. Assoc./AMMSA  
Mail Code SD47, Bldg. 4481  
Marshall Space Flight Center, AL 35812  
Phone: 256-544-9196  
Fax: 256-544-2102  
alex.chernov@msfc.nasa.gov

**Dr. James Kaduk, ICDD Rep.**

BP-Amoco Research Center  
150 W. Warrenville Road  
MC F-9, P.O. Box 3011  
Naperville, IL 60566-7011  
Phone: 630-420-4547  
Fax: 630-420-5252  
kadukJA@BP.com

**Members, continued**

**Howard M. Einspahr (03)**

Macromolecular Crystallog.  
Bristol-Myers Squibb  
P.O. Box 4000, H23-03  
Princeton, NJ 08543-4000  
Phone: 609-252-5267  
Fax: 609-252-6030  
howard.einspahr@bms.com

**Kathryn R. Ely (03)**

The Burnham Institute  
10901 N. Torrey Pines Rd.  
La Jolla, CA 92037-1062  
Phone: 858-646-3135  
ely@burnham.org

**James A. Kaduk (04)**

BP Chemicals  
150 W. Warrenville Road  
P.O. Box 3011, MC F-9  
Naperville, IL 60566  
Phone: 630-420-4547  
Fax: 630-420-5252  
kadukja@bp.com

**Katherine Kantardjieff (03)**

Dept. of Chem and Biochem  
California State U.-Fullerton  
800 N State College  
Fullerton, CA 92834-9480  
Phone: 714-278-3752  
Fax: 734-939-4225  
kkantardjieff@fullerton.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 (02)**

Department of Geosciences  
SUNY Stony Brook  
Stony Brook, NY 11794-2100  
Phone: 631-632-8196  
Fax: 631-632-8240  
john.parise@sunysb.edu

**Jeffrey E. Post (02)**

Department of Mineral Sciences  
Smithsonian Institution  
Washington, DC 20560-0119  
Phone: 202-357-4009  
Fax: 202-357-2476  
post.jeffrey@nmnh.si.edu

**John C.H. Spence (02)**

Dept. of Physics and Astronomy  
Arizona State University  
Tempe, AZ 85287-1504  
Phone: 480-965-6486  
Fax: 480-965-7954  
spence@asu.edu

**Ronald E. Stenkamp (04)**

Depy of Biological Structure &  
Biomolecular Structure Center  
University of Washington  
Box 357420,  
Seattle, WA 98195-7420  
Phone: 206-685-1721  
Fax: 206-543-1524  
stenkamp@u.washington.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 Committee**

**Bill Duax (02)**

Hauptman-Woodward M R I  
73 High Street  
Buffalo, NY 14203-1196  
Phone: 716-856-9600  
Fax: 716-852-4846  
duax@hwi.buffalo.edu

**Ex-Officio Voting Members  
ACA Council (2002)**

**Charles Carter, President**

Dept. of Biochem and Biophys  
U. of North Carolina Chapel Hill  
CB7260, Chapel Hill, NC 27599-7260  
Phone: 919-966-3263  
Fax: 919-966-2852  
carter@med.unc.edu

**Raymond E. Davis, V-President,**

Dept. of Chem. & Biochem.  
The University of Texas at Austin  
Austin, TX 78712-1167  
Phone: 512-471-4440  
Fax: 512-471-8696  
redavis@mail.utexas.edu

**Douglas Ohlendorf, Treasurer**

Dept. of Biochem, Mol Biol & Biophys  
University of Minnesota  
Rm 6-155 JachH, 1214,321 Church St. S.  
Minneapolis, MN 55455  
Phone: 612-624-8436  
Fax: 612-624-5121  
ohlend@cdiff.med.umn.edu

**Ex-Officio Non-Voting Members**

**BCST Co-Chairs:**

**Alice P. Gast (03)**

Stanford University  
Dept of Chem. Engineering  
381 North South Mall, Keck Bldg.  
Room 279, Stanford, CA 94305-5025  
Tel: 650-725-3145; Fax: 650-725-7294  
alice@chemeng.stanford.edu

**Kenneth N. Raymond, NAS (02)**

University of California, Berkeley  
Department of Chemistry  
Berkeley, CA 94720-1460  
Tel: (510)-642-7219; Fax: (510)-486-5283  
raymond@socrates.berkeley.edu

\*Send NRC/BCST correspondence to

**Douglas J. Raber, NRC/BCST Director**

2101 Constitution Avenue, NW  
Washington, DC 20418  
Tel.: 202-334-2156; Fax: 202-334-2154  
draber@nas.edu

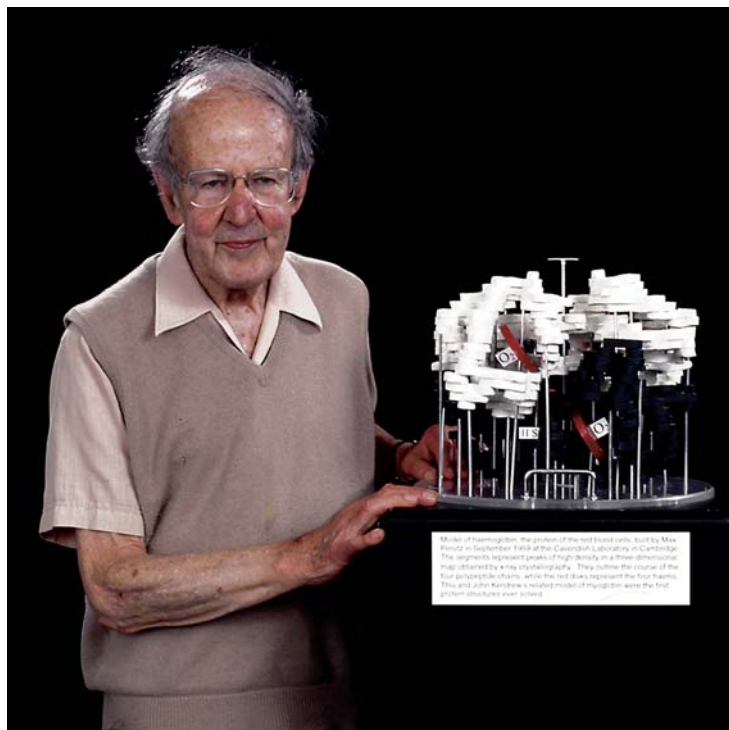
**NRC STAFF**

**Tamae Maeda Wong, Prog. Dir.**

Board on International Sci. Org.  
National Research Council  
2101 Constitution Avenue, NW,  
Room NAS 246,  
Washington, DC 20418  
Phone: 202-334-2243  
Fax: 202- 334-2231  
twong@nas.edu

**Valerie Theberge, Sr Prog. Ass't.**

Board on International Sci. Org.  
National Research Council  
2101 Constitution Avenue, NW,  
Room NAS 246  
Washington, DC 20418  
Phone 202-334-1785  
Fax: 202-334-2231  
vtheberge@nas.edu



Model of haemoglobin, the protein of the red blood cells, built by Max Perutz in September 1958 at the Cavendish Laboratory in Cambridge. The segments represent peaks of high density in a three-dimensional map obtained by x-ray crystallography. They follow the course of the four polypeptide chains, whose side chains represent the four haemes. This and John Kendrew's related model of myoglobin were the first protein structures ever solved.

**Max Perutz (1914 - 2002)**

Early on Wednesday, 6th February, Max Perutz died of cancer after a long and productive life. Starting a Ph.D. in 1936 under J.D. Bernal at the Cavendish Laboratory, he applied X-ray crystallography to proteins and in 1953 developed the method of isomorphous replacement using heavy atoms to solve the phase problem. This led to the solution of the first protein structures, those of myoglobin by his colleague John Kendrew and his collaborators, and of haemoglobin by Perutz and his collaborators. For this, Perutz and Kendrew were awarded the 1962 Nobel Prize for Chemistry. With a great deal more work during the 1960's, Perutz and his colleagues went on to solve the atomic structures of both oxy- and deoxy-haemoglobin which allowed him to propose a stereochemical mechanism for the cooperative binding of oxygen to haemoglobin. Max was the first author of a recent review (Ann. Rev. Biophysics and Biomolecular Structure 1998) of cooperativity in haemoglobin in which he noted that his mechanism still appeared to be correct.

In more recent years, he worked on ligand binding to haemoglobin to help develop a clinically useful drug for increasing oxygen delivery to hypoxic tumours for radiation therapy, and to infarcted tissues. He also developed a strong interest in the structure of the polyglutamine tracts in Huntington's disease. In his youth, as a sideline, he also worked on glaciers. He studied the transformation of snowflakes that fall on glaciers into the huge single ice crystals that make up its bulk, and the relationship between the mechanical properties of ice measured in the laboratory and the mechanism of glacier flow. He was a prolific and talented writer of popular articles and book reviews, many published in the New York Review of Books. He also wrote a number of books, including "Is Science Necessary" and "I Wish I'd Made You Angry Earlier" which are collections of essays. "Science is Not a Quiet Life" published by World Scientific Publishing is essentially his scientific autobiography.



**Max with Jeanne Perry at a gathering in David Eisenberg's back yard when he visited their UCLA laboratory in 1991.**

At the Cavendish Laboratory with the support of Professor Lawrence Bragg and with his first Ph.D. student, John Kendrew, who joined him in 1945, he built up a group working on the molecular structure of biological systems which grew to four people in 1950 and to about 40 people by 1960. Merging then with other groups from Cambridge and London to create the MRC Laboratory of Molecular Biology on the Hills Road site (now Addenbrooke's) in 1962, he became Chairman of the new Laboratory until 1979 when he "retired." Since then he has worked nearly every day in the Laboratory which has grown to house over 400 people. Over the years, the Laboratory has been a prolific source of discoveries and inventions. In addition to his own research achievements, Max will be remembered for his interest in and warm support of the work of others, and as one of the founders of Molecular Biology.

*from the web site statement of the  
MRC Laboratory of Molecular Biology*

Professor Sir George Radda, Chief Executive of the Medical Research Council, said: "Our heartfelt sympathies go out to his family at this difficult time. Not only have his colleagues, at the MRC and in the scientific community lost a great co-worker and friend, but Britain and the world will be mourning the loss of one of the 20th century's scientific giants."

"The impact of Max's work remains a foundation on which science is being undertaken today. His Nobel Prize winning work on protein structure is more relevant now than ever as we turn attention to the smallest building blocks of life to make sense of the human genome and mechanisms of disease."

"Max had many interests and a great love of music and will be remembered as much for his science as for his endless drive and passion for knowledge and better communication of research. He was recognised as a great communicator himself. His books and book reviews stand up as good literature as well as good science."

“He was still working on research projects and publishing work in his 80s. Once asked why he didn’t retire at 65 he said he was tied up in some very interesting research at the time. This sums Max up well. He continued as a ‘retired’ worker after 1979, publishing over 100 papers and articles during his retirement. Until the Friday before Christmas, he was active in the lab almost every day, submitting his last paper just a few days before then.”

“He has inspired countless young scientists and encouraged them to communicate their research in plain language to those whose lives are changed through their work. He will be sorely missed, but his life and work will continue to shape science and motivate new generations to understand the way the body functions and how this will help us manage health and disease.”

*from the MRC statement on his death*

**Deane K. Smith**  
(1930 - 2001)

Deane Smith was a long time member of both the ACA and the ICDD. He was ACA secretary from ACA 1976 to 1978 and his ICDD history included Distinguished Fellow since 1995, 16-year board member, and Chairman of the Board 1978-1982 and 1986-1990. Deane co-founded and became the first Editor-in-Chief for the journal *Powder Diffraction*, a position that he held for thirteen years (1986-1999). Deane nurtured and grew both the ICDD and *Powder Diffraction* into strong international organizations through a fantastic blend of technical knowledge, leadership, and interpersonal skills. Deane also served as a primary instructor at the ICDD’s X-ray diffraction clinics, since 1991. In his capacity as a member of the Organizing Committee of the Denver X-ray Conference, Deane contributed his expertise in developing dynamic conference programs for the education of the XRD and XRF communities.

He was a Fellow of the Geological Society of America and the Mineralogical Society of America and was elected to the Commission on Powder Diffraction of the International Union of Crystallography for 1993-96. He also served on the Joint Committee on Powder Diffraction Standards.

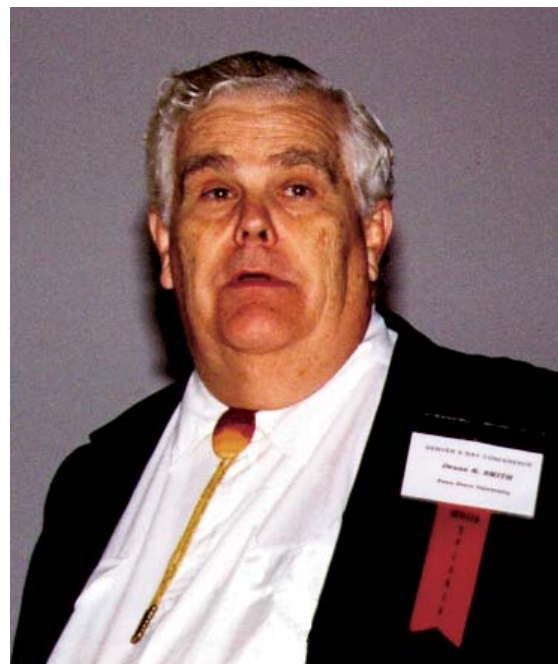
He will be sorely missed by the scientific community and the hundreds of scientists, teachers, and students that he influenced

*from the note circulated to ICDD members*

Deane K. Smith Jr., 70, of State College, PA died Friday, Sept. 7, 2001, at home. Born Nov. 8, 1930, in Berkeley, Calif., he was a son of the late Deane K. Sr. and Anna Virginia Long Smith. On July 24, 1953, in St. Louis Park, Minn., he married Patricia Ann Lawrence, who survives at home.

In 1952, he graduated from California Institute of Technology with a bachelor’s degree in geology and in 1956, he graduated from the University of Minnesota with a doctorate in geology. From 1956-60, he was a research associate of the Portland Cement Association Fellowship at the National Bureau of Standards in Washington, D.C. During the 1960s, he worked as a chemist in the Inorganic Materials Division of the Lawrence Radiation Laboratory in California and later as assistant section leader of the lab’s Properties of Materials section.

In 1968, he joined Penn State’s Department of Geosciences as an associate professor and became professor in 1971. Following 27 years of teaching and research, he was professor emeritus of mineralogy at Penn State. During his career, he published many papers and won



numerous awards, including the C.S. Barrett Award in Diffraction Analysis for lifetime achievement in X-ray diffraction. A newly discovered mineral, deanesmithite, was named after him. He taught many summer short courses in X-ray diffraction, was past chairman of International Center for Diffraction Data, organized many scientific conferences, was the first editor for the Journal of Powder Diffraction and was a mentor to colleagues and students. Locally, he was known for his gemology class at Penn State. He was also adviser to the Nittany Valley Gem and Mineral Club. As proprietor of the Gem Dugout, he became a worldwide source for X-ray diffraction needs.

In addition to his wife, he is survived by three daughters, Paula Lynn Smith of Seattle, Jeanette D. Metcalf of Chesterland, Ohio, and Sharon R. Stanford of Colbran, Colo.; two sons, Kingsley L. of Madison, Wis., and Dana E. of State College; and nine grandchildren.

*from the State College Centre Daily Times*



*Don C. Wiley (1944 – 2001)*

The crystallographic world suffered a huge loss with the untimely death of Don Wiley, who disappeared mysteriously from Memphis on 15 November 2001 to be found weeks later downstream in the Mississippi river. This tragedy is felt acutely by his family and immediate associates; but the pain spreads to us who knew Don less directly and on to many others who understand biology better because of him. Don drew fame from his impact in biology, but his drive to solve central problems in biology had an under-appreciated influence on crystallography as well.

As best I can recall, I first met Don in the summer of 1971 at a Cold Spring Harbor Symposium. This was a watershed meeting held just as macromolecular crystallography was reaching its stride. Don was there to present his thesis work with Bill Lipscomb on the 5.5Å structure of aspartate transcarbamylase (ATCase), and this lanky, long-haired young man cut a striking figure. Expressing familiar graduate-student anxiety, he sported a purpose-made T-shirt featuring his subject, ATCase, ensnared in the blind alleys of a maze and labeled “There is no law that says ... things must get better.” Indeed, it was left to successors in Lipscomb’s laboratory to find the way out to atomic-level resolution and to show the basis for allosteric regulation in this classic enzyme.

At least for me, however, Wiley had already left a mark with his first paper. In elegant crystallographic reasoning he deduced the molecular symmetry of ATCase (published with Lipscomb in *Nature*, as were so many to follow). He crystallized this oligomeric

protein in two lattices for which he determined crystal densities; one was found to have a third of the molecule in the asymmetric unit of a trigonal space group and the other to have half in the asymmetric unit of a tetragonal space group. The minimal (and ultimately correct) point-group symmetry of ATCase was deduced thereby to be  $D_3$  (32). I use this example in my crystallography course to this day.

I next recall encountering Wiley a few years later at a protein crystallography conference in the Berkshires. Don talked about the beginnings of his work with John Skehel on influenza virus, giving one of his patently lucid descriptions of complicated biology. Wiley had realized ahead of other crystallographers that extra-membranous fragments of membrane proteins could be tractable and was able to crystallize the exterior portion of flu hemagglutinin. In later solving this structure, he and Ian Wilson used three-fold averaging to resolve the phasing from a single derivative. This work provided a highly influential demonstration of the power of non-crystallographic symmetry. The structure itself was also a marvel, recapitulating the tall and slender form of its discoverer; and hemagglutinin proved all the more remarkable when the structure as transformed to its low-pH state came out some years afterward. This dramatic conformational change continues to provide a mechanistic paradigm for cellular entry by HIV and other fusogenic viruses.

In membrane ectodomain encores, Wiley subsequently tackled surface glycoproteins from trypanosomes and major histocompatibility complex (MHC) molecules from antigen-presenting cells. He was highly decorated for the latter work, winning both a Lasker Award and the Japan Prize with his collaborating colleague Jack Strominger. I remember learning about this fascinating problem from Pam Bjorkman at her Gordon Conference poster describing packing in Class I MHC crystals, and when her structure appeared I was awestruck by its message -- an ‘Aha’ structure if ever I saw one. Soon afterward, I was asked by a colleague to help him study aspects of peptide presentation by MHC molecules and to present our results at a meeting of prominent molecular immunologists. On reading background literature, I learned that much was already known ahead of Wiley’s work and feared that I had misjudged the impact of the structure. My first impressions were reinforced resoundingly at the meeting, however; nearly every talk featured a picture of the Class I structure with its ‘extra density’ assigned to antigen peptides.

Wiley continued to attack important problems in molecular immunology and virology. The list is long: envelope glycoproteins from HIV, herpes and Ebola viruses as well as other hemagglutinin variants; Class II MHC molecules, T-cell receptors, Natural Killer (NK) receptors, various peptide processing factors, and so on. The problems that he chose often posed technical challenges. Technology often develops best when driven by such challenges, and the crystallographic problems in Wiley’s laboratory motivated new instruments and techniques. Thus, Wiley together with his close colleague Steve Harrison fostered the building of a new electronic area detector and already had a prototype in use for the Class I MHC structure (1987) to complement synchrotron data from extremely thin crystals (also non-standard at the time). In further development of the in-house detector system, crystal freezing was introduced. This proved to be essential in extending the trypanosomal surface protein structure to an atomic-level (1990), and cryoprotection technology was then perfected into a routine tool for other radiation-sensitive problems at Harvard and ultimately around the world.

Don was an undergraduate in physics and chemistry at Tufts University and earned his Ph.D. in Biophysics at Harvard University (with Lipscomb

in 1971) after which he immediately joined the faculty of the Department of Biochemistry and Molecular Biology at Harvard, where he spent his entire career apart from a sabbatical year in England. In 1987 he became an Investigator with the Howard Hughes Medical Institute and in 1990 he also became associated with Children's Hospital in Boston. He was a member of the National Academy of Science and the American Philosophical Society and a fellow of the American Academy of Arts and Sciences. He was recognized by other major honors including the Louisa Gross Horwitz Prize and the Gairdner Award as well as the Lasker Award and Japan Prize noted above. Don is survived by his wife Katrin and their two children and by two children from a previous marriage.



*Cold Spring Harbor Symposium -- Summer 1971*

My admiration for Don Wiley and his scientific accomplishments is immense. He used structure to define biology when others were content just to see structures. He focused on the truly important and derived stirring insights from his studies; but he had the intellectual discipline to stay within the bounds of his data. His results have redefined whole fields. His lectures were paragons of clarity. He was the life of the party. We miss him sorely.

*Wayne A. Hendrickson*

***We gratefully acknowledge the continued support of ACA CORPORATE MEMBERS***

*American Magnetics*  
[www.americanmagnetics.com](http://www.americanmagnetics.com)

*Douglas Instruments Limited*  
[www.douglas.co.uk](http://www.douglas.co.uk)

*Protein Data Bank*  
[www.rcsb.org/pdb](http://www.rcsb.org/pdb)

*Area Detector Systems Corp.*  
[www.adsc-xray.com](http://www.adsc-xray.com)

*Emerald BioStructures*  
[www.emeraldbiostructures.com](http://www.emeraldbiostructures.com)

*Protein Solutions*  
[www.protein-solutions.com](http://www.protein-solutions.com)

*ATPS Inc.*  
[www.atpsinc.com](http://www.atpsinc.com)

*Gilson Inc. Cyberlab*  
[www.gilson.com](http://www.gilson.com)

*Rheometric Scientific Inc.*  
[www.protein-solutions.com](http://www.protein-solutions.com)

*Bibliothek Technische Hochschule  
Hannover, Germany*

*Hampton Research*  
[www.hamptonresearch.com](http://www.hamptonresearch.com)

*Rigaku/MSc, Inc.*  
[www.RigakuMSc.com](http://www.RigakuMSc.com)

*Blake Industries, Inc.*  
[blake4xray@worldnet.att.net](mailto:blake4xray@worldnet.att.net)

*International Centre  
for Diffraction Data*  
[www.icdd.com](http://www.icdd.com)

*Schneider Electrical  
Technologies, Inc.*  
[schneideret@cs.com](mailto:schneideret@cs.com)

*Bruker/Nonius*  
[www.bruker-axs.com](http://www.bruker-axs.com)

*MAR-USA, Inc.*  
[www.mar-usa.com](http://www.mar-usa.com)

*Syrrx, Inc.*  
[www.syrrx.com](http://www.syrrx.com)

*Cambridge Crystallographic  
Data Centre*  
[www.ccdc.cam.ac.uk](http://www.ccdc.cam.ac.uk)

*Microsource*  
[www.bede.com/micro.html](http://www.bede.com/micro.html)

*UOV/Biblioteca Universitaria  
Oviedo, Spain*

*Charles Supper Company, Inc.*  
[www.supper.com](http://www.supper.com)

*NeuroProbe*  
[www.neuroprobe.com](http://www.neuroprobe.com)

*Wyatt Technology Corp.*  
[www.wyatt.com](http://www.wyatt.com)

*Compaq Computer Corp.*  
[www.compaq.com](http://www.compaq.com)

*Osmic, Inc.*  
[www.osmic.com](http://www.osmic.com)

*X-Ray Research GmbH*  
[www.marresearch.com](http://www.marresearch.com)

*Cryo Industries of America, Inc.*  
[www.cryoindustries.com](http://www.cryoindustries.com)

*Oxford Cryosystems*  
[www.oxfordcryosystems.com](http://www.oxfordcryosystems.com)

*Crystal Logic Inc.*  
[www.xtallogic.com](http://www.xtallogic.com)

*Oxford Instruments Inc.*  
[www.oxford-instruments.com](http://www.oxford-instruments.com)

## Crystallography Web Watch

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

**ACA Web Site** — During the past year, the ACA web site has undergone a needed facelift. The redesigned site is brighter and more inviting. It's also much easier to navigate within the updated site. If you haven't already done so, check it out: <http://www.hwi.buffalo.edu/ACA/>

**Doug Powell's Crystallography Page** — Doug does a good job collecting information on topics such as publication information, organizations, databases, crystallography e-mail lists, crystallography education and general interest, etc. Check out the links section, in particular: <http://www.msg.ukans.edu/~xraylab/links.html>

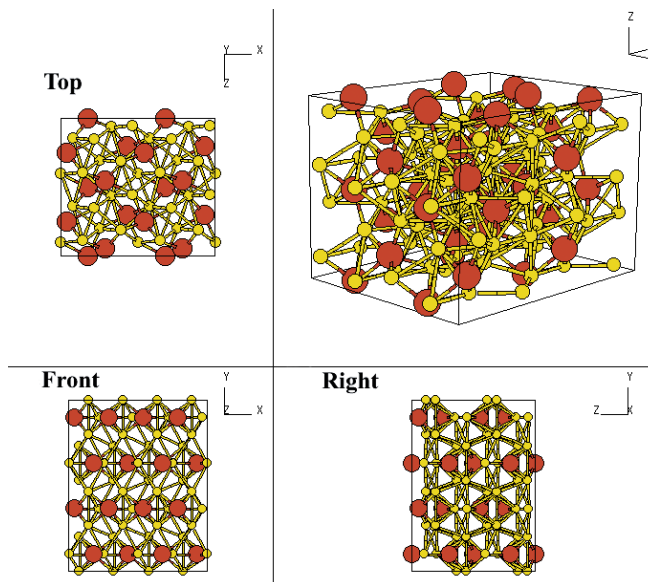
**Inorganic Structures** — The Naval Research Laboratory maintains a database of the crystal structures of common inorganic phases, including alloys. The database can be indexed by space group, Pearson symbol or prototype. Color pictures of each of the phases in various orientations are accessible online, and the Cartesian coordinates can be downloaded for off-line, interactive viewing or calculations on your own computer: <http://cst-www.nrl.navy.mil/lattice/>

**FASEB** — The Office of Public Affairs of the Federation of American Societies for Experimental Biology advances a number of activities designed to promote biological and biomedical sciences and allow researchers to be heard when governmental regulations are being developed. Their web site provides links to illustrated essays on breakthroughs in bioscience. The essays are generally written in a lively fashion and would be a great resource when your non-scientist friends ask you to explain, for instance, the polymerase chain reaction: <http://www.faseb.org/opar/break>

**Powerpoint Presentations** — It seems like everyone is now using Microsoft Powerpoint to present their work at meetings and conferences. One of the great powers of these presentations is that they can become more than just "slide shows" by adding animation and multimedia, for example. A good place to look for ideas to spice up your next Powerpoint presentation is the computer tips web site: <http://www.computertips.com/Microsoftoffice/MsPowerPoint/aheader.html>

**"Molecular animation"** — You've probably seen those rotating molecules in a presentation. There are a number of programs available to create animations, but you can do it yourself by creating a series of molecular images, each rotated by 5 or 10°, using a drawing program, such as MolScript: <http://www.avatar.se/molscript/>. The individual images can be pasted together into a movie using a program, such as the SGI routine makemovie, and inserted it into a Powerpoint slide.

... and don't forget to check out the web page for the XIX Congress of the IUCr which takes place this August in Geneva, Switzerland: <http://www.kenes.com/iucr/index.html>



*Cementite ( $DO_{11}Fe_3C$ )  
from the Inorganic Structures site*

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

### Bionet Crystallography

The [bionet.crystallography](mailto:bionet.crystallography) electronic newsgroup is a useful electronic resource for biological crystallography, providing a forum for general discussion, and a place to post notices such as job advertisements or synchrotron beamline availability. However, in the past year this resource has become a disgraceful collection of spam. To rectify the situation, I have agreed to become moderator of the newsgroup, which means that spam is deleted by me rather than posted to the group. This relatively minor (but satisfying!) task will be made more rewarding if the intended audience--the crystallographic community--makes more active use of the newsgroup again. To subscribe (i.e., receive posts by e-mail) or to browse recent messages, see [www.bio.net](http://www.bio.net). To post messages, send e-mail to: [xtal-log@net.bio.net](mailto:xtal-log@net.bio.net).

Cathy Lawson

## *Call for Proposals for Synchrotron Beamtime at the Structural Biology Center Beamlines at the Advanced Photon Source*

The Structural Biology Center (SBC) at Argonne National Laboratory Advanced Photon Source announces that both the insertion-device and bending magnetic beamlines are fully available for user research. The SBC invites from the user community proposals for beamtime at its national user facility for macromolecular crystallography. The SBC Collaborative Access Team (CAT) located at APS sector 19 operates an insertion-device beamline, 19ID, and a bending-magnet beamline, 19BM. Both beamlines are equipped with a fully tunable monochromator designed to reach most absorption-edge energies (19ID: 6.5 – 19.0 KeV and 19BM: 6.5 – 13 KeV) routinely used in macromolecular crystallography and X-ray optics designed to deliver a stable, intense, highly focused X-ray beam with low angular divergence onto protein crystal samples. The crystal environment includes a *kappa* geometry goniostat, high-resolution long distance microscopes, cryogenic crystal coolers, high sensitivity fluorescence detectors, and a low noise 210 x 210 mm CCD detector. The insertion device beamline is ideally suited for

very challenging projects such as: small, weakly diffracting crystals, projects having very large unit cells, ultra-high resolution structures and MAD/SAD experiments. The bending magnetic beamline is ideally suited for those projects requiring very accurate MAD/SAD measurements. Data can be processed with HKL2000, MOSFILM or d\*TREK. Crystallographic software to analyze MAD data is available to users. Beamtime on the 19ID and 19BM beamlines are available to the crystallographic research community via a peer reviewed proposal system. The proposal evaluation is based upon the projects' scientific merit, need for synchrotron time at the SBC facility, feasibility of conducting the experiments at the SBC, and the probability of success of the project. Proposals will be accepted on continual bases.

Additional information and proposal submission forms can be obtained from the SBC web site (<https://www.sbc.anl.gov>). For further information, please contact **Stephan L. Ginell**, Ph.D., User Program Coordinator, at [ginell@anl.gov](mailto:ginell@anl.gov) or 630-252-3972.

---



### *Ira Flatow to Receive Wood Award*

Ira Flatow will receive the Elizabeth A. Wood award at the San Antonio ACA meeting in May. The award was established in 1997 to honor Betty Wood, a crystallographer at Bell Labs until her retirement, President of ACA in 1957, and the author of “*Crystals and Light*,” and “*Science From Your Airplane Window*.” The award is given to those who excel in bringing science to the attention of a wider audience.

Ira Flatow is currently host of NPR’s “*Talk of the Nation. Science Friday*.” He is also president of *ScienCentral, Inc.*, a company dedicated to increasing the amount of science news shown on television. He has authored two charming books about science: “*Rainbows, Curveballs : And Other Wonders of the Natural World Explained*,” Wm Morrow & Co., 1988; and “*They All Laughed : From Light Bulbs to Lasers : The Fascinating Stories Behind the Great Inventions That Have Changed Our Lives*,” HarperCollins, New York, 1992. He maintains a “*Bookshelf*” on the *Science Friday* website and the **Books** column in this *Newsletter* lists selections from it – see pages 27-30.

Flatow was science reporter for *CBS This Morning* program (1989-90), host and writer of the Emmy Award science series *Newton’s Apple* (1982-87) on PBS and veteran science correspondent for National Public Radio’s *All Things Considered* and *Morning Edition* (1971-1987). Ira also hosted a four part PBS environmental series: *Earthkeeping*. Readers of publications such as *TV Guide*, *Woman’s Day*, *Science Digest* and *The Los Angeles Times* (among others) are also familiar with his articles and comments on various

scientific subjects. Viewers of the TV show *PM Magazine* will recall his memorable “*Halley’s Comet*” story. Because of his love of marine tropical fish, Ira currently writes a column for hobbyists about “reef keeping” for the *Aquarium Fish* magazine.

Online service is being added to the list of Flatow’s accomplishments. His science interviews can be heard on *The Discovery Channel* web page. He is currently putting *Science Friday* on the Internet with the idea of creating a unique presence for science and technology reachable by students and adults. *Science Friday Kids Connection* has recently joined *Science Friday* to create a place where students can exchange ideas with scientists online.

His broadcasting career goes back to his days in high school. A native New Yorker, Ira got his first taste of television news working on a morning high school TV news program. When he entered college, in 1967, to study for his engineering degree (SUNY Buffalo, 1971) Ira began working in radio at WBFO, Buffalo. While his first news assignments involved antiwar demonstrations and riots, his first real science stories took shape during Earth Day in 1970. He was news director of the station by the time he left to join the fledgling National Public Radio in Washington, DC.

Ira Flatow is a board member of the National Association of Science Writers and a double winner of the AAAS-Westinghouse science award, the only person to win for both radio and television in one year. He lives with his wife, Miriam, and children Sam, Anna and Abigail in Connecticut.

*from the NPR scifri website*

### *Deadline Extended for Summer School Proposals*

The call for proposals for hosting the **ACA X-Ray Summer Course** (ACAXRSC) has been extended until May 15<sup>th</sup>. This course has been organized and hosted by the University of Georgia (UGA) since summer 1997; it was initiated in 1992 and hosted at the University of Pittsburgh 1992-1996. The school has normally run continuously for about two weeks, including weekends. At UGA, we spent 7 days on fundamental (small molecule) crystallography and 5 days on macromolecular crystallography with one day of rest between the two sessions. There were morning and evening lectures with hands-on laboratory in the afternoon. We tried to have unusual or special evening lectures, for example when Bob Sweet demonstrated long distance control of an experiment at the Brookhaven synchrotron facility. The organization is flexible and should be adjusted to suit local needs and desires. Critical factors are: (1) to have readily accessible and well-equipped lecture rooms, (2) to provide access to modern equipment for use by course participants and (3) to arrange for enough lecturers to cover the entire span of modern single-crystal X-ray crystallography.

The ACA website has complete details about how proposals should be structured as well as a description of the requirements, including lecture and laboratory facilities, housing, travel, food services, and budget. See also the *Fall 2001 Newsletter* for the first *Call for Proposals* and a *History of the School* by Bob Sparks. The extended, May 15<sup>th</sup> deadline will still allow those submitting proposals to meet with the ACA Council for discussions if they plan to attend the San Antonio meeting. Completed proposals, including contact information, should be sent to: **Dr. Gary Newton**, Univ. of Georgia, Biochem. and Molec. Biol. Dept., Life Sciences Bldg., Athens, GA 30601; newton@chem.uga.edu; tel.706-542-3272; fax: 706-542-3077.



### *Ira Flatow's Book List:*

Ira Flatow, who is to receive the Elizabeth A. Wood Award (see page 25) has a Book List that can be reached from the NPR *Talk of the Nation: Science Friday* website, or more directly at: <http://www.npr.org/programs/scifri/flatow.html>. His list is extensive, and for the most part consists of books that have been discussed on his *Science Friday* show. Book titles are linked to the *Amazon.com* site so that editorial reviews, etc. are readily accessible. The following were selected from recently published books in this list, with descriptions selected from the *Amazon.com* link.

***The Accelerating Universe : Infinite Expansion, the Cosmological Constant, and the Beauty of the Cosmos*** by Mario Livio. John Wiley and Sons, 2000. (Discussed Aug 2001.) "Livio, who helps direct research conducted with the Hubble Telescope, ..... explains how the latest data are straining the long-standing assumptions of cosmologists, who are now forced to contemplate a universe in which the energy in empty space is unexpectedly dominating matter in pushing the galaxies toward frigid oblivion. Far more than a puzzle for specialists, the struggle to re-interpret the cosmos raises fundamental questions about the human craving for order: Does this craving reflect deep cosmic harmonies that helped create our species? Or does it simply defy an irreducible chaos that we would rather not confront? ..." (Bryce Christensen, for *Booklist*, American Library Assoc.)

***A Passion for DNA: Genes, Genomes, and Society***, by James D. Watson. CSHL Press, 2000. (Discussed Jun 2000.) "A collection of essays written for a variety of occasions during the past three decades. Watson concentrates on three themes: his autobiography; the growth, practice, and application of molecular biology; and the contemporary ethos of science. he describes his growth and maturation as a scientist and administrator; the meaning of success in science; science and public policy; the nature of cancer research; the past, present, and future of DNA; and the Human Genome Project and its bioethical problems." (Donald A. Chambers, for *The New England Journal of Medicine*, August 3, 2000)

***Absolute Zero and the Conquest of Cold***, by Tom Schachtman. Houghton Mifflin, 1999. (Discussed Jan 2000.) "Writing for a general audience, science writer Schachtman surveys the history of scientific manipulation of cold, beginning in the 1600s with an alchemist who air conditioned a portion of West Minster Abbey. His story includes coverage of the invention of thermometers and scales, the beginnings of the field of thermodynamics, the 19th-century ice trade, the use of coolants in the production of microchips, and the current pursuit of absolute zero." (*Book News, Inc.*®, Portland, OR)

***Blue Frontier: Saving America's Living Seas***, by David Helvarg. W H Freeman & Co, 2001. (Discussed Apr 2001.) "A text showing how informed people can make a difference in the fight to protect and restore the oceans surrounding the Americas and other world oceans. Discusses the current problems of pollution, overfishing and other damaging effects of industrialization on our oceans, and how they can be remediated." (Amazon.com Book Info --DLC: Marine resources conservation--United States.)

***Copenhagen***, by Michael Frayn. Anchor Books, 2000. (Discussed Oct 2000.) "...Copenhagen is an explosive re-imagining of the mysterious wartime meeting between two Nobel laureates to discuss the atomic bomb. In 1941 the German physicist Werner Heisenberg made a clandestine trip to Copenhagen to see his Danish counterpart and friend Niels Bohr.....the two men were on opposite sides in a world war. Why Heisenberg went to Copenhagen and what he wanted to say to Bohr are questions that have vexed historians ever since. In Michael Frayn's ambitious, fiercely intelligent, and daring new play,

Heisenberg and Bohr meet once again to discuss the intricacies of physics and to ponder the metaphysical—the very essence of human motivation." (Amazon.com book description.)

***Cracking the Genome: Inside the Race to Unlock Human DNA***, by Kevin Davies. Free Press, 2001. (Discussed Jan 2001.) "Drawing on his own genetics expertise and interviews with key scientists including Francis Collins, J. Craig Venter, Eric Lander, Kari Stefansson, and John Sulston, the author (science writer and *Current Biology* editor) describes the intense competition between public and private researchers to complete the process of mapping the human genome sequence." (*Book News, Inc.*®, Portland, OR.)

***Database Nation: The Death of Privacy in the 21st Century***, by Simson Garfinkel. O'Reilly, 2000. (Discussed Jan 2000.) "Forget the common cold for a moment. Instead, consider the rise of "false data syndrome," a deceptive method of identification derived from numbers rather than more recognizable human traits. Simson Garfinkel couples this idea with concepts like "data shadow" and "datasphere" in *Database Nation*, offering a decidedly unappealing scenario of how we have overlooked privacy with the advent of advanced technology." (E. Brooke Gilbert for Amazon.com.)

***Decoding Darkness: The Search for the Genetic Causes of Alzheimer's Disease***, by Rudolph Tanzi and Ann Parsons. Perseus Publishing, 2000. (Discussed Jul 2001.) "...Chronicles the struggle to find causes and a possible cure for Alzheimer's disease, centering on the search for the gene responsible for the production of a renegade protein, beta amyloid. Offers a portrait of the high stakes of molecular genetics, the revolution that propels it, the obstacles that threaten to derail it, and the families whose lives depend on it. Tanzi teaches neurology at Harvard Medical School and directs the Massachusetts General Hospital's Genetics and Aging Unit. Parson is a science journalist." (*Book News, Inc.*®, Portland, OR)

***Einstein in Love: A Scientific Romance***, by Dennis Overbye. Viking Press, 2000. (Discussed Oct 2000.) "...An acclaimed science writer's insightful and revelatory biography of young Einstein—teenager in love, draft dodger, bohemian, poet, and scientist—drawing upon many unpublished letters and years of research." (Amazon.com book description.)

***Eclipse: Voyage to Darkness and Light***, by David Levy. Ibooks, 2000. (Discussed Jan 2001.) "David Levy's personal account of the 1999 solar eclipse. As Levy tells of his journey to the event, his observations and reactions to it, he relates the fascinating history of solar eclipses and explains why they happen and what results from them." (Amazon.com book description)

***Earth Odyssey: Around the World in Search of Our Environmental Future***, by Mark Hertsgaard. Broadway Books, 2000. (Discussed Jun 2000.) "The author, a respected journalist, traveled the world for six years to understand the effect of pollution on people living with deforestation, drought, famine, and air pollution. He reports on the global environmental predicament through the eyes of people who live with it, politicians and peasants, taxi drivers and activists." (*Book News, Inc.*®, Portland, OR)

***Elegant Universe: Superstrings, Hidden Dimensions, and the Quest for the Ultimate Theory***, by Brian Greene. W.W. Norton, 1998. (Discussed Feb 1999.) "Greene, originator of groundbreaking discoveries in superstring theory, describes

exciting new research in the field and discusses implications for the future of science. Using plain language with no math or technical jargon, he tells how superstring theory identifies nature's fundamental building blocks, which turn out to be, not subatomic particles, but vibrating strands whose vibrational patterns account for all of nature's forces. He combines everyday examples, b&w diagrams, and a sense of fun to illustrate complicated concepts." (*Book News, Inc.*®, Portland, OR)

**"Flight: My Life In Mission Control,"** by Chris Kraft. E. P Dutton, 2001. (Discussed May 2001. "...The Right Stuff meets Rocket Boys in this gripping memoir by the man who helped create some of the greatest moments in U.S. space history." (Amazon.com book description.)

**"Genome: The Autobiography of a Species in 23 Chapters,"** by Matt Ridley. HarperCollins, 2000. (Discussed Feb 2000.) "...Ridley provides a quick, clear guide to the few words and concepts he must use to translate hard science into English. His writing is informal, relaxed, and playful, guiding the reader so effortlessly through our 23 chromosomes that by the end we wish we had more. He believes that the Human Genome Project will be as world-changing as the splitting of the atom; if so, he is helping us prepare for exciting times--the hope of a cure for cancer contrasts starkly with the horrors of newly empowered eugenicists. Anyone interested in the future of the body should get a head start with the clever, engrossing Genome." (Rob Lightner for Amazon.com.)

**"Living Terrors: What America Needs to Know to Survive the Coming Bioterrorist Catastrophe,"** by Michael Osterholm and John Schwartz. Delacorte Press, 2000. (Discussed Apr 2001) "...A former Minnesota State epidemiologist and a science reporter for *The Washington Post* claim that a terrorist attack with viral or bacterial agents is inevitable. Their measures for safety pivot around training medical staff and stocking emergency rooms rather than, for example, stop making everyone so mad at us." (*Book News, Inc.*®, Portland, OR)

**"Human Natures: Genes, Cultures, and the Human Prospect,"** by Paul R. Ehrlich. Island Press, 2000. (Discussed Oct 2000.) "Why do we behave the way we do? Biologist Paul Ehrlich suggests that although people share a common genetic code, these genes "do not shout commands at us . . . at the very most, they whisper suggestions." He argues that human nature is not so much the result of genetic coding; rather, it is heavily influenced by cultural conditioning and environmental factors. With personal anecdotes, a well-written narrative, and clear examples, *Human Natures* is a major work of synthesis and scholarship as well as a valuable primer on genetics and evolution that makes complex scientific concepts accessible to lay readers." (Amazon.com book description.)

**"Memory: From Mind to Molecules,"** by Eric Kandel. W H Freeman & Co, 2000. (Discussed Oct 2000.) "...What is memory and where in the brain is it stored? How is memory storage accomplished? These key questions are addressed in *Memory*, the first book for a general readership to offer an up-to-date, comprehensive overview of memory from molecules and cells to brain systems and cognition." (Amazon.com book description.)

**"Nine Crazy Ideas in Science,"** by Robert Ehrlich, Princeton University Press, 2001. (Discussed Aug 2001.) "...Makes several eccentric scientific theories accessible to general readers and, more important, it teaches methods of evaluating new ideas so we can decide for ourselves whether or not they make sense."

(J.B. Peck for Amazon.com.)

**"Mosquito: A Natural History of Our Most Persistent and Deadly Foe"** by Andrew Spielman Sc.D., Michael D'Antonio. Hyperion, 2001. (Discussed Jul 2001.) "Spielman and D'Antonio (Harvard University's senior investigator in tropical diseases and Pulitzer Prize-winning *Newsday* reporter, respectively) examine the life of the mosquito, the mosquito's intimate relationship with human beings and how an understanding of this relationship has changed our understanding of disease, the dangers posed by mosquitoes, and what methods are used to confront these adaptable, clever, and relentless insects." (*Book News, Inc.*®, Portland, OR)

**"One Universe: At Home in the Cosmos,"** by "Charles Liu, Neil DeGrasse Tyson, and Robert Irion". Joseph Henry Press, 2000. (Discussed Feb 2000.) "...Explores the physical principles that govern the workings of our own world to appreciate how they operate in the cosmos around us. Shows how the physical principles that operate in our kitchens and backyards are actually down-to-Earth versions of cosmic processes. ...The book is being published in conjunction with the opening of the new \$200million Rose Center for Earth and Space at the American Museum of Natural History with the new Hayden Planetarium as its centerpiece." (Amazon.com book description.)

**"Shots in the Dark: The Wayward Search for an AIDS Vaccine,"** by Jon Cohen. WW Norton, 2001. (Discussed Feb 2001.) "...Based on the complex technical, political, and ethical barriers to developing an AIDS vaccine which he chronicles, a California writer for *Science* magazine advocates a coordinated Manhattan Project-type effort by basic and applied researchers, business interests, and US government policymakers. Cohen concludes on the semi-hopeful note that, unlike the situation a decade ago, the world is now watching. Includes a glossary of medical terms." (*Book News, Inc.*®, Portland, OR)

**"The Age of Spiritual Machines: When Computers Exceed Human Intelligence,"** by Ray Kurzweil. Scholastic, 2000. (Discussed Mar 2000.) "...His book ranges widely over such juicy topics as entropy, chaos, the big bang, quantum theory, DNA computers... neural nets, genetic algorithms, nanoengineering, the Turing test, brain scanning... chess-playing programs, the Internet--the whole world of information technology past, present, and future. This is a book for computer enthusiasts, science fiction writers in search of cutting-edge themes, and anyone who wonders where human technology is going next." (*The New York Times* Book Review, Collin McGinn)

**"The Big Idea: 150 Years of the Best and Worst Ideas of Modern Science,"** by David Levy (editor). ibooks, 2001. (Discussed Aug 2001.) "This fascinating new book, based on *Scientific American's* wildly popular feature, "50, 100, and 150 Years Ago in Science Today", presents the often hilarious human aspect of science as well as a serious timetable of scientific discovery. (Amazon.com book description.)

**"The Botany of Desire: A Plant's-Eye View of,"** by Michael Pollan. Random House, 2001. (Discussed Jul 2001.) "...Pollan has read widely on the subject and elegantly combines literary, historical, philosophical, and scientific references with engaging anecdotes, giving readers much to ponder while weeding their gardens." (Shawn Carkonen for Amazon.com's Best of 2001.)

**"The Eternal Darkness: A Personal History of Deep-Sea Exploration,"** by Robert Ballard. Princeton University Press, 2000. (Discussed June 2000.) "...The clarity of the prose never lets you down, though the story gets into ever more complex tales of

equipment, exploration, science and political maneuvering.” (The *New York Times* Book Review, Michael Parfit.)

**“The Expanded Quotable Einstein,”** by Alice Calaprice. Princeton University Press, 2000. (Discussed Oct 2000.) “Much more than a series of soundbites, this book of documented quotations and supplementary information about Einstein’s life, family, and work puts his thoughts into context. A fairly complete biographical account of this multifaceted man emerges--as son, husband, father, lover, scientist, philosopher, aging widower, humanitarian, and friend. It shows us vividly why the real and imagined Einstein continues to fascinate people the world over.” (Amazon.com book description.)

**“The Monk in the Garden: The Lost and Found Genius of Gregor Mendel,”** by Robin Marantz Henig. Houghton Mifflin, 2000. (Discussed Sep 2000.) “...On the singular facts of Mendel’s life, *The Monk in the Garden* makes easy reading. But as a larger effort to represent Mendel to 21st-century readers, it is deficient.” (The *New York Times* Book Review, Joe Cain.)

**“The Mystery of the Aleph: Mathematics, the Kabbalah, and the Human Mind,”** by Amir Aczel. Four Walls Eight Windows, 2000. (Discussed Jan 2001.) “...An engaging, pellucid explanation of the mathematical understanding of infinity, enlivened by a historical gloss on age-old affinities...” (Washington Post Book World, 11/19/2000.)

**“The Runaway Universe: The Race to Discover the Future of the Cosmos,”** by Donald Goldsmith. Perseus Press, 2000. (Discussed Oct 2000.) “...After reviewing recent findings that the universe is not just expanding but is doing so ever faster, popular astronomer Goldsmith chronicles the scientific race to determine the crucial cosmic parameters that will reveal the rate of expansion and therefore the universe’s age and ultimate fate. The rush is not so much that the world might end suddenly while people were between insurance policies, but that the scientists who come up with credible and enduring numbers first win fame and grants.” (*Book News, Inc.*®, Portland, OR)

**“The World’s Water 2000-2001: The Biennial Report on Freshwater Resources,”** by Peter Gleick. Island Press, 2000. (Discussed Aug 2000.) “Gleick (of the nonprofit organization, the Pacific Institute for Studies in Development, Environment, and Security, Oakland) offers a report on the state of the world’s water, debates surrounding it, and the technology that has the potential to address some of the most troubling problems associated with it. Of likely use to water resource professionals in government agencies and nongovernmental organizations, researchers, students, and concerned citizens.” (*Book News, Inc.*®, Portland, OR)

**“Zero: The Biography of a Dangerous Idea,”** by Charles Seife. Viking, 2000. (Discussed Mar 2000.) “..The Babylonians invented it, the Greeks banned it, the Hindus worshipped it, and the Christian Church used it to fend off heretics. Seife, a US correspondent for the international magazine *New Scientist*, follows the number zero from its birth as an Eastern philosophical concept to its struggle for acceptance in Europe and its apotheosis as the mystery of a black hole. He describes the work and thought of scholars, mystics, and cosmologists as they battled over the meaning of this mysterious number.” (*Book News, Inc.*®, Portland, OR)

## Contributors / Exhibitors ACA '02

**We are grateful to the following organizations and institutions whose generous contributions help to make the ACA meeting a success**

*ACS Petroleum Research Fund*

*BioCryst Pharmaceuticals, Inc.*

*Hampton Research Corp.*

*Hoffmann-La Roche Inc.*

*International Centre for Diffraction Data*

*Merck Research Laboratories*

*Pharmacia Corporation*

*Rigaku/MSC, Inc.*

*Structural GenomiX, Inc.*

**Be sure to visit with our good friends the exhibitors during the meeting**

*Area Detector Systems Corp.*

*Beevers Miniature Models*

*Blake Industries, Inc.*

*Bruker/Nonius*

*CCP4*

*Cambridge Crystallographic Data Center*

*Cartesian Technologies*

*Corning Incorporated*

*Diversified Scientific, Inc.*

*EDAX/TSL*

*Gilson, Inc.*

*Greiner Bio-One, Inc.*

*Hampton Research*

*MAR-USA, Inc.*

*Molecular Dimensions, Inc.*

*Oxford Cryosystems, Inc.*

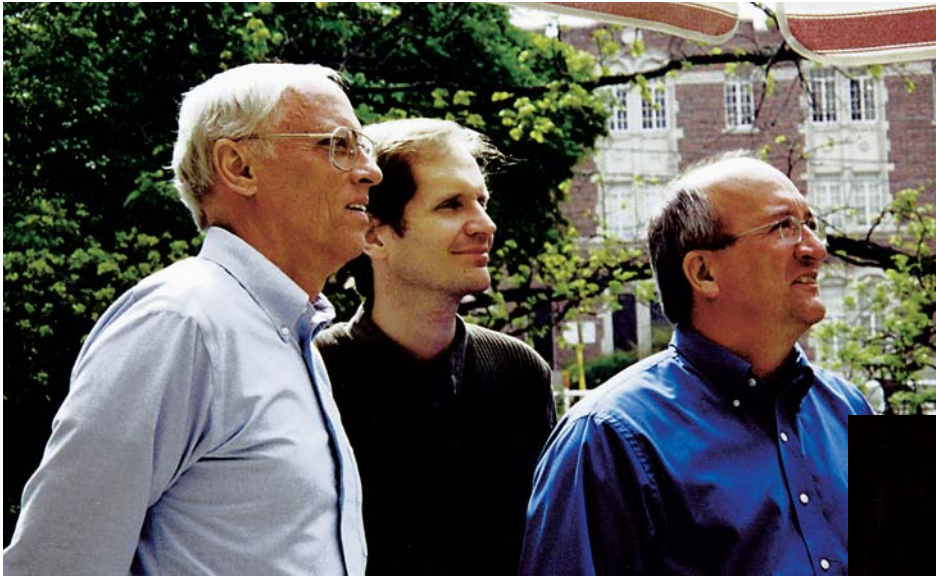
*Oxford Instruments*

*Protein Data Bank*

*Rigaku/MSC, Inc.*

*Rigaku/Osmic, Inc.*

*Wyatt Technology Corp.*



**ACA 2002 in San Antonio, TX, May 25-30**

The program for San Antonio emphasizes several distinct themes beyond the normal diverse spectrum of sessions and reports. A workshop, the *Transactions* sessions, and several other sessions all fit together under the umbrella of structures and material science as probed by powder methods. A two-day minisymposium on *Crystal Engineering* will include an impressive line-up of international speakers. Also, since this is a joint meeting with the AACG, there will be four sessions dedicated to crystal nucleation and growth topics. And there is a multi-day program on **electron crystallography** and **electron microscopy** also with many international speakers.

Wally Cordes ([wcordes@mail.uark.edu](mailto:wcordes@mail.uark.edu)), above left and Travis Gallagher ([travis.gallagher@nist.gov](mailto:travis.gallagher@nist.gov)), center, are Co-Program Chairs; Co-Local Chairs Ray Davis, ([redavis@mail.utexas.edu](mailto:redavis@mail.utexas.edu)), and Marv Hackert ([m.hackert@mail.utexas.edu](mailto:m.hackert@mail.utexas.edu)), are making plans at the table. *Marv is on right in both pictures.*

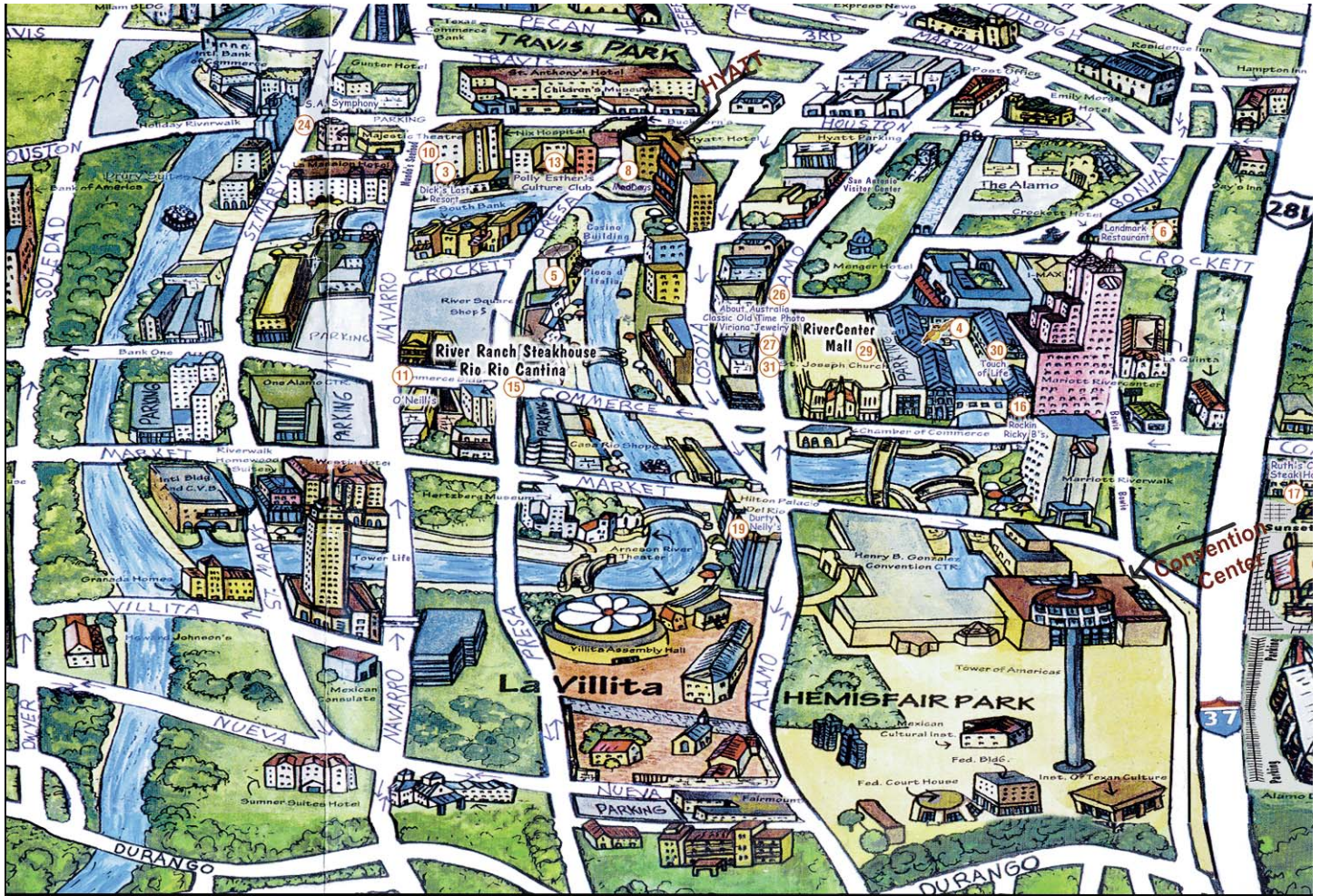
*Right: Bill Duax, Marcia Evans, Bill Stallings and Marv Hackert in front of the Alamo, May, 2001, before the Council meeting*



San Antonio, the Alamo City, is the most popular tourist destination in Texas. The Hyatt Regency is located downtown on the Riverwalk, a charming area with many restaurants which is only a few blocks from the Convention Center. Check out the Institute of Texas Culture, which is close to the Convention Center, and well worth visiting. For more information see the Convention Center and Visitor's Bureau web site: [www.sanantoniocvb.com](http://www.sanantoniocvb.com).

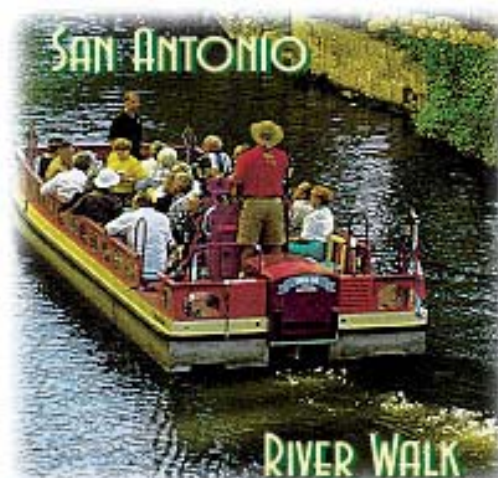
*At right: Casa Rio on the Riverwalk.*





*Above: Downtown San Antonio. arrows indicate the Hyatt Hotel and the Henry B. Gonzales Convention Center.*

*Below, the Rivercenter, a river cruise around downtown, and a local mission.*



## Hands-On Workshop; Non-Merohedral Twinning at Texas A&M University

May 23-24, 2002

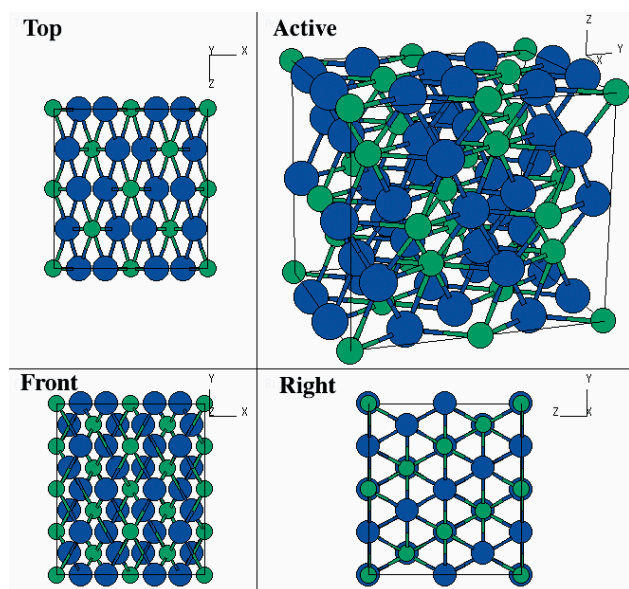
The Data, Standards, and Computing Committee will sponsor a two-day, hands-on workshop in practical non-merohedral twinning methods at Texas A&M University immediately before the 2002 annual meeting in San Antonio. This workshop will be held on May 23-24, 2002, which will allow participants to attend other regularly scheduled workshops at the meeting site beginning May 25th.

This workshop will focus on methods instead of theory. Several diffractometers will be available for data collection during the workshop. Experts committed to attending include Regine Herbst-Irmer, Simon Parsons, and Victor Young. All participants are encouraged to bring their own problem samples and data. For more information about the workshop site please see <http://www.chem.tamu.edu/xray/>.

The number of participants will be limited to 20 in order to make this a productive time for all involved. A nominal fee of \$50 will provide coffee and snacks for breaks, as well as delivered lunches near the workshop site. A block of rooms at several reasonably priced hotels has been reserved. All necessary details for accommodations will be provided to participants by email.

Texas A&M University is approximately 120 miles from San Antonio. Participants are encouraged to fly into San Antonio and take rental cars for the remainder of the scenic trip to College Station, TX. The organizers will assist in pairing participants for ride sharing.

The organizers are **Victor Young: [young@chem.umn.edu](mailto:young@chem.umn.edu)**, (612-625-6897) and **Joe Reibenspies: [reibenspies@mail.chem.tamu.edu](mailto:reibenspies@mail.chem.tamu.edu)**, (979-845-9125). Please contact Victor Young by May 1, 2002 for registration and lodging details.



TiSi<sub>2</sub>(C54)

from *Inorganic Structures* website, see page 19

## Gordon Research Conference: Diffraction Methods in Structural Biology

Connecticut College, New London, Connecticut  
July 14-19, 2002

This biennial conference has, for many years, had the reputation as the premier conference focusing on development of diffraction methods for elucidating bio-molecular structure. One focus will be on the bottlenecks of high-throughput structure determination. Another emphasis will be functional and mechanistic interpretation, including the integration of structure with sequence mechanical and quantum mechanical computations. Seating is limited to 135 participants. Early registration is encouraged. All Conferees are encouraged to submit Poster Abstracts. A selection of Poster Presenters will be invited by Session Chairs to do mini-talks.

For further information, please visit the Gordon Conference site [www.grc.uri.edu](http://www.grc.uri.edu). or contact one of the Conference Co-Chairs, Michael Chapman: [chapman@sb.fsu.edu](mailto:chapman@sb.fsu.edu) or Tom Terwilliger: [terwill@telomere.lanl.gov](mailto:terwill@telomere.lanl.gov).

**Tonya Kilpatrick**, Coordinator Institute of Molecular Biophysics Florida State University Tallahassee, FL 32306-4380 Tel: (850) 644-7632 email: [tkilpat@sb.fsu.edu](mailto:tkilpat@sb.fsu.edu)

## Addendum to the Meeting Report on 59 Pittsburgh Diffraction Conference, held Oct 25-27, 2001

The names of some of the speakers were inadvertently left out of the Winter, 2001 meeting report. (Photographs were subtitled with names, but not all the speakers were present when the *Newsletter* photographs were taken.)

Speakers in the 'Exotic Uses of the CCD in Non-Standard Crystallographic Investigations' symposium were: Susan Byram, Dieter Schwarzenbach, Simon Parsons, Maren Pink, Chuck Campana, Joe Reibenspies, Przemyslaw Dera, Jonathan Hanson, Tim Graber, Philip Coppens, Alan Pinkerton, Joe Ferrara. Victor Young, Alan Pinkerton, and John Parise were Co-organizers.

Speakers in the 'Intra- and Intermolecular Interactions' symposium in memory of George Jeffrey were: Alfred French, Stanley Nyburg, Dieter Mootz, Ned Seeman, B.C. Wang, Sine Larsen, John Rosenberg, Paul Baures, Christer Aakeroy, Robin Rogers, Lee Brammer, John Ruble, Larry Shapiro, John Finney, Dave Stout, Jonathan Parquette, Helen Berman, Martin Caffrey, Carol Brock, Michael Zaworotko, Yong Xiong, Miguel Garcia-Garibay, Bin Du, Anna Gudmundsdottir. The Co-organizers were Bryan Craven and Jeanette Krause Bauer.

A special thank you to Stanley Nyburg for regaling us with stories about George and Maureen Jeffrey. It made for an interesting and enjoyable banquet evening.

Jeanette Krause Bauer,  
PDS President & Conference Chair

## Meeting Calendar

### MAY 2002

- 23-24 **Hands-On Workshop; Non-Merohedral Twinning**, Texas A&M University, College Station, TX.
- 25-30 **American Crystallographic Association Annual Meeting, ACA-2002**, San Antonio, TX.

### JUNE 2002

- 7-12 **Electron Crystallography School 2002**, Tampere, Finland.
- 10-14 **2002 ICDD X-ray Clinics: Advanced Methods in X-ray Powder Diffraction**, ICDD Headquarters, Newtown Square, PA.
- 21-21 **6 International School and Symposium on Synchrotron Radiation in Natural Sciences**, Jaszowiec, Poland.
- 21-21 **11 Annual Fibre Diffraction and Non Crystalline Diffraction Meeting**, Keele University, Staffordshire, England.
- 27-27 **The (first) American Conference on Neutron Scattering (ACNS)**, Knoxville, TN. See the website or contact: Rob Briber, University of Maryland, rbriber@eng.umd.edu or Julie Borchers, NIST, julie.borchers@nist.gov or Paul Butler, ORNL, butlerpd@ornl.gov
- 24-26 **Time-Resolved Chemistry: From Structure to Function**, Manchester, UK.

### JULY 2002

- 7-11 **SPIE conference on "Advances in Neutron Scattering Instrumentation"** Seattle, WA. See <http://spie.org/info/am/>
- 14-19 **International Conference on the Physics and Chemistry of Ice**, Newfoundland, Canada.
- 14-19 **Gordon Research Conference: Diffraction Methods in Structural Biology**, Connecticut College, New London, CT.
- 29-02 **Denver X-ray Conference**, Denver, CO.

### AUGUST 2002

- 4-6 **Crystal Chemistry of New Materials & Soft Matter Studied by Synchrotron & Neutron Diffraction**. ESRF-ILL Grenoble are organizing this satellite meeting preceding the main IUCr-Geneva Congress.

- 4-6 **Neutron and Synchrotron X-Ray Scattering in Condensed-Matter Research (NSCmr2002)**. Paul Scherrer Institut, Villigen, Switzerland.

- 6-15 **IUCr XIX - XIX Congress and General Assembly of the International of Crystallography**, Geneva, Switzerland. Joel Bernstein, Chair, Organizing Committee, joel@bgumail.bgu.ac.il; Menahem Kaftory, Chair, Program Committee, kaftory@technix.technion.ac.il. See [www.iucr@kenes.com/iucr/](http://www.iucr@kenes.com/iucr/) and also [www.geneva-tourism.ch](http://www.geneva-tourism.ch) and [www.unige.ch/crystal/ahdf/geneva02.html](http://www.unige.ch/crystal/ahdf/geneva02.html).

- 22-26 **International Workshop on Photoionization**, Hyogo, Japan.

- 25-29 **12 International Conference on Small Angle Scattering**, Venice, Italy.

- 29-31 **The forth international congress "Natural glasses: glasses in geosciences, environmental sciences and archeometry**, Lyon, France.

### SEPTEMBER 2002

- 4-6 **Synchrotron Radiation in Polymer Science II**, Sheffield, UK. Sponsored by the European Physical Society, Macromolecular Group.

- 4-7 **6 International Conference on Quasielastic Neutron Scattering**, Potsdam (near Berlin), Germany.

- 8-12 **Chemistry towards Biology**, Portoroz, Slovenia. Organized by the Slovenian Chemical Society with the sponsorship of the Federation of European Chemical Societies.

- 10-14 **XTOP 2002 6 biennial conference on High Resolution X-Ray diffraction and Topography**, Grenoble-Aussois, France.

### OCTOBER 2002

- 7-9 **29 Annual Stanford Synchrotron Radiation Laboratory Users' Meeting**, Menlo Park, CA.

### JUNE 2003

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

### JULY 2003

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

- 26-31 **American Crystallographic Association Annual Meeting, ACA 2003**, Cincinnati, Ohio.

### AUGUST 2003

- 10-13 **AsCA'03/Crystal-23**, Cable Beach Club resort, Broome, Western Australia.

- 14-15 **Workshop on Biological Structure**, Cable Beach Club resort, Broome, Western Australia.

- 14-19 **Sagamore Meeting** run by the IUCr Commission on Charge, Spin and Momentum Densities, Cable Beach Club resort, Broome, Western Australia.

- 24-30 **21 European Crystallographic Meeting**, Durban, South Africa

### SEPTEMBER 2003

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

### JUNE 2004

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

#### Contributors to this issue:

Dan Anderson, Charles Carter, Wally Cordes, Lachlan M.D. Cranswick, William I.F. David, Michael Deem, William Duax, Marcia Evans, Ira Flatow, Judith Flippin-Anderson, Travis Gallagher, Steve Ginell, Marvin Hackert, Richard Henderson, Wayne Hendrickson, Jim Kaduk, Tonya Kilpatrick, Jeanette Krause Bauer, Cathy Lawson, Armel Le Bail, Helen McDonnell, Kay Onan, John Parise, Joe Reibenspies, Frank Rotella, Earle Ryba, Jack Sack, Peter Stephens, Hideo Toraya, Maryjane Tremayne, Robert Von Dreele, Winnie Wong-Ng, Leihai You, Victor Young.

## 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/](http://www.hwi.buffalo.edu/ACA/)

### Crystallographer-FT/PT

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

## POSITIONS PREVIOUSLY LISTED

### Protein Crystallographer - Tenure Track

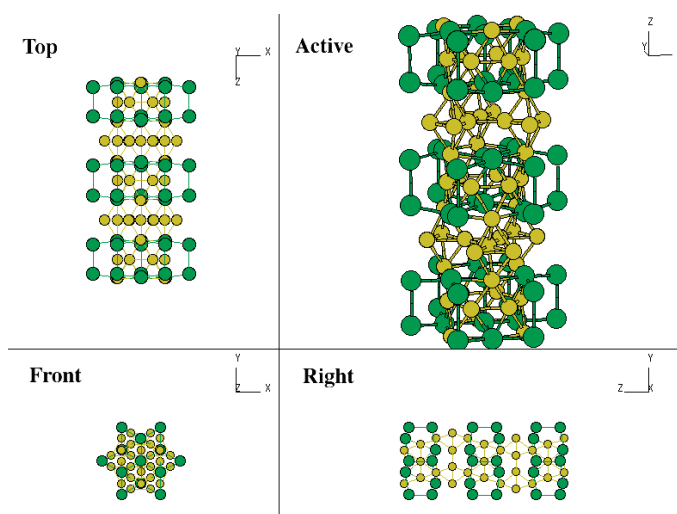
Applications are invited for a tenure-track, full-time faculty appointment at the Assistant or Associate Professor level in the Institute of Materials Science and Department of Molecular and Cell Biology at the University of Connecticut. Applicants must have a doctorate degree in a biochemical, chemical or biophysical field and postdoctoral experience. The research area of interest is X-ray crystallography of proteins or protein/nucleic acids complexes, which will complement current research strengths in structural biology. The successful candidate will teach undergraduate and graduate courses in the Department of Molecular and Cell Biology and will be affiliated with the Polymer Program of the Institute of Materials Science. The successful candidate will be expected to establish a productive, extramurally funded research program. A part of the 28-member Department of Molecular and Cell Biology will soon expand into a new building adjacent to the Institute. The Institute is an interdisciplinary research facility that houses the 14-member Polymer Program and the X-ray diffraction facilities. The anticipated starting date is August, 2002. To apply, submit curriculum vitae, a brief statement of

research and teaching interests, and arrange to have three letters of recommendation sent to: Search Committee #2, Institute of Materials Science, University of Connecticut, 97 North Eagleville Road, U-3136, Storrs, CT 06269-3136. Review of applications will begin after publication of this notice and will continue until the position is filled. We encourage applications from under-represented groups, including minorities, women and people with disabilities. (Search #02A170)

### Macromolecular Crystallographer/Data-Processing and Programming Specialist:

Area Detector Systems Corp. (ADSC) has an immediate opening for a Research Scientist with background experience in Molecular Crystallography and qualified in computer programming. The successful candidate will contribute to research on advanced software requirements used to analyze fine slice data used in the advancement of protein crystallography. This requires at least three years experience in Molecular Crystallography coupled with solid knowledge of C++ programming. Experience obtained either as a graduate student or in Post-Doctorate work is applicable.

ADSC is a privately held company founded in 1981 and is located in the sunny southern California area near San Diego. The company is an industrial leader that develops and manufactures CCD Detectors that are used in Synchrotrons worldwide in Protein Crystallography applications. Most recently, it has considerably increased the research and development activity with the support of major government grants. The company's web site is [adsc-xray.com](http://adsc-xray.com). Send your resume outlining your experience to: ADSC (c/o T.H. Hontz), 12550 Stowe Drive, Poway, CA, 92604 or e-mail to [sales@adsc-xray.com](mailto:sales@adsc-xray.com).



*C<sub>36</sub> (Hexagonal Laves)*

*from Inorganic Structures website, see page 19*