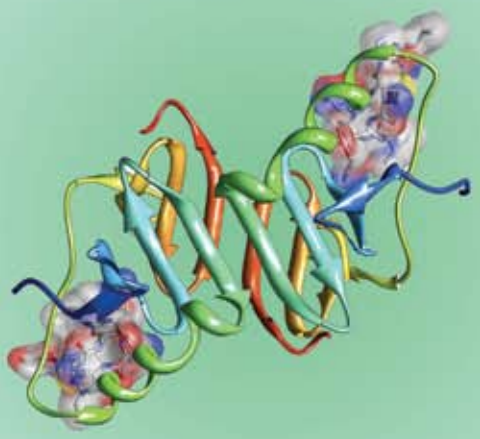
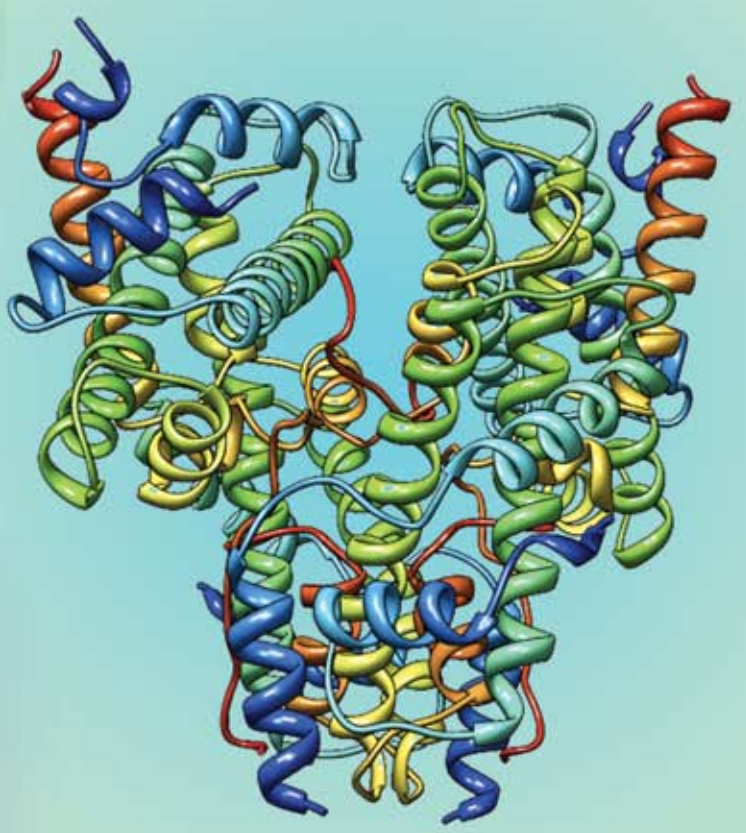
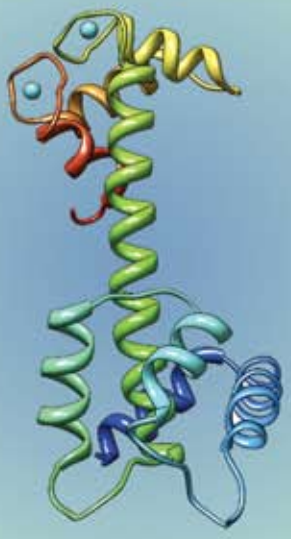
ACA RefleXions

American Crystallographic Association

Number 1
Spring, 2008







The Patterson Award at the 2008 ACA Meeting in Knoxville, TN

Bruker AXS

X8 PROSPECTOR ULTRA

Perfect for Protein Screening and High Quality Structures

The X8 Prospector ULTRA features the ultra-low-maintenance IμS source and the photon-counting ÅXIOM 200 detector to achieve the ultimate combination of performance and convenience. From high-speed screening to SAD phasing, the ULTRA outperforms conventional rotating anode systems, producing higher data quality in a fraction of the time. Simple to operate and maintain, the ULTRA is the perfect tool for the home laboratory or for off-line screening at the beamline.

- Ultra-reliable and extremely stable micro-focus sealed source with new Quazar optics for a surprisingly high intensity; superior to a 5 kW conventional rotating anode with multilayer optics
- ÅXIOM 200 digital photon-counter for ultimate detector sensitivity and speed
- Virtually no maintenance and low cost of ownership; completely air-cooled, 3 year tube lifetime guaranteed

Contact us for more details and a system demonstration! www.bruker-axs.com

American Crystallographic Association

ACA RefleXions

ACA HOME PAGE: **www.AmerCrystalAssn.org**

Cover: see page 19. Images from Bi-Cheng Wang's career in crystallography. B.C. is to receive the 2008 Patterson Award at the Knoxville ACA Meeting.

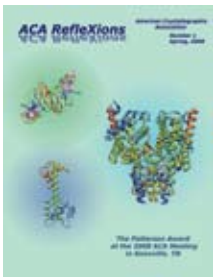


Table of Contents

Contributions to ***ACA RefleXions*** may be sent to either of the Editors:

Connie (Chidester) Rajnak
4210 Old Field Trail
Kalamazoo, MI 49008
tel. 269-342-1600
fax 716-898-8695
conniechidester@earthlink.net

Judith L. Flippen-Anderson
3521 Launcelot Way
Annandale, VA 22003
tel. 703-346-2441
fax 716-898-8695
flippen@rscb.rutgers.edu

Please address matters pertaining to advertisements, membership inquiries, or use of the ACA mailing list to:

Marcia J. Colquhoun, Director of Administrative Services
American Crystallographic Association
P.O. Box 96, Ellicott Station
Buffalo, NY 14203-0906
tel: 716-898-8692; fax: 716-898-8695
marcia@hwi.buffalo.edu

Deadlines for contributions are: February 1 (Spring), May 1 (Summer), August 1 (Fall) and November 1 (Winter)

ACA RefleXions (ISSN 1058-9945) Number 1 2008. 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. POST-MASTER: Send address changes to ACA, P.O.Box 96, Ellicott Station, Buffalo, NY, 14205-0096.

BRUKER

Bruker AXS

APEX DUO
Versatility
Dual wavelength! High-resolution data and absolute configuration from organic molecules in one experiment.

APEX II ULTRA
Brilliance
The best Mo flux density and best beam quality when performance really matters.

KAPPA APEX II
SMART APEX II
Gold Standard
The most trusted systems for chemical crystallography. Reliable, high-precision instrumentation.

SMART X2S
Automation
The first fully automated benchtop system for crystallography. Fully air-cooled and low maintenance. 3-D structures at the touch of a button.

SMART BREEZE
Low Maintenance
Air-cooled option provides great performance and minimal installation requirements.

You Provide the Challenge
We Provide the Solution

We have tailored a wide variety of solutions to meet your needs in chemical crystallography. The combination of high-performance goniometers and X-ray sources, the fastest and most sensitive detectors, and intuitive software ensures that you get the results you expect, quickly and reliably.

Contact us for more details and a system demonstration! www.bruker-axs.com

think forward

Crystallography

President's Column:

Greetings and best wishes for 2008! This year should be another exciting and challenging year - the ACA in Knoxville in June and the IUCr in Osaka in August!

First let me offer my congratulations to Bob Von Dreele (Argonne) and Jim Britten (McMaster) who join the ACA Council as VP and Canadian Representative, respectively. Congratulations as well to all the SIG representatives elected to serve this year. I also wish to express our collective thanks to Alan Pinkerton for his dedication and leadership as President of the ACA last year. We are lucky to have Alan with us on the Council this year, but will miss Bob Bau as he rotates off Council. Bob led us in Hawaii, and guided and entertained us in Salt Lake City. Thanks - Bob!

One of the benefits of serving on your ACA Council is the opportunity to see all the work done behind the scenes by our staff in Buffalo and the many volunteers across the country that make the ACA function. Of course the culmination of much of this effort is bringing you our annual meeting. This year the annual meeting is early because of the IUCr meeting in Osaka in August. We hope that many of our members will be able to attend both conferences. Our meeting will be in Knoxville from May 31 - June 5. Local Chair Jason Hodges and Program Co-Chairs Paul Butler and Dean Myles have put together a great meeting and program (**http://neutrons.ornl.gov/conf/aca2008/**).

One of the reasons for meeting in Knoxville is to be near the new ultra-high-intensity (1.4MW) Spallation Neutron Source (SNS). The SNS is the first of a new generation of spallation neutron user facilities and is source of the world's most intense pulsed neutron beams for diffraction, small-angle scattering, and spectroscopy. The SNS plus the recently upgraded High Flux Isotope Reactor (HFIR) neutron source make Oak Ridge a premier global center for neutron science. On Sunday evening, June 1st, ACA attendees and their guests will have an opportunity to take a field trip to Oak Ridge National Laboratory to tour of the Spallation Neutron Source and enjoy a reception with hors d'oeuvres and refreshments. For security reasons, pre-registration is required so be sure to go to our web site and sign up for this event.

It was impressive to see Paul Butler and Dean Myles work with the SIG representatives in Salt Lake City to shape the program for this year's meeting. Four workshops will be offered on Saturday, May 31st, including one on neutron macromolecular crystallography and another on small angle scattering. This year the *Transactions* Symposium will focus on "Complementary Methods to Crystallographic Techniques for Structure/Function studies of Biological Macromolecules." It will be a pleasure to present B.C. Wang with the Patterson Award in Knoxville. The BioMac SIG is organizing a session in B.C.'s honor on Wednesday, June 4th. The Etter Early Career Award goes to Radu Custelcean of Oak Ridge National Laboratory. Congratulations to both B.C. and Radu on their awards.

However, for many of us the ACA annual meeting is much more than a great program and award presentations. It is a time to see the latest advances in instrumentation, catch up with old colleagues and to make new friends. I was an ORTEP junkie in the '60s and remember the thrill of meeting Carroll Johnson in New Orleans at my first ACA meeting in 1970. Of course, ACA meetings were smaller in those days, but I wish there were ways we could provide a similar experience for the graduate students who attend our meeting in Knoxville. I encourage you to bring your students and postdocs to the meeting, and I encourage everyone to make all the younger crystallographers feel welcome.

Here are some other meetings to add to your calendar: The ACA School on Small Molecule Crystallography will be held July 7-16, and the IUCr triennial meeting will be in Osaka, Japan from August 23–31. The 8th Ewald Prize will be presented to David Sayre (Stony Brook) during the Opening Ceremony in Osaka. Next year's ACA meeting will also have an international flare since we will be meeting July 25-30 in Toronto (Jim Britten is Program Chair), then back to Chicago in 2010 (July 22-31), to New Orleans in 2011 (May 19–28) and to Boston in 2012. Finally, largely through the efforts of Chris Hill, we managed to make last year's meeting in Salt Lake City climate neutral. You can find out more about this and our efforts to make our 2008 ACA Meeting Climate Neutral on the ACA web site.

I look forward to working for, and with, all of you over the coming year as your President – it is indeed an honor. I encourage members to contact me, or any member of Council, with your ideas for improving the operation of the ACA or our annual meeting. One change to look for is that at the Knoxville meeting you will be given a choice of receiving the abstracts in either book or CD format. When elected VP a year ago, I thought I had a lot of time to prepare for my year as President and this first column - my how time flies. I would be remiss if I did not include a special thank you to four very special people who help make this job a lot easier and the ACA run so smoothly - Bill Duax and Marcia Colquhoun from the Buffalo office, and Judith Flippen-Anderson and Connie (Chidester) Rajnak (both former ACA Presidents) who edit our excellent newsletter *RefleXions*. Also, my thanks and appreciation to all Council members and the dozens of volunteers who make the ACA my favorite scientific organization.

I hope to see you all in Knoxville. Remember, the advanced registration deadline is April 4th.

Marv Hackert

Correction: The editors regret that **Abe Clearfield's** name was inadvertently left out of the list of donors published in the winter 2007 *RefleXions*. He has generously donated to the **Buerger; Fankuchen; Patterson; Trueblood; Warren; Etter Early Career**; and **Supper Instrumentation Awards** as well as to the **Pauling Poster Prize**; the **Student Travel Fund** and the **Latin America Initiative**.

David Sayre To Receive 8th Ewald Prize

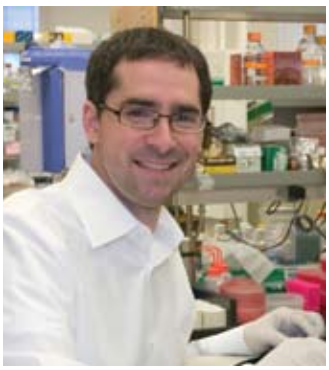
The IUCr is pleased to announce that **David Sayre**, Department of Physics, State University of New York, Stony Brook, has been awarded the eighth **Ewald Prize** *for the unique breadth of his contributions to crystallography, which range from seminal contributions to the solving of the phase problem to the complex physics of imaging generic objects by x-ray diffraction and microscopy, and for never losing touch with the physical reality of the processes involved*. The presentation of the Ewald Prize will be made during the Osaka Congress Opening Ceremony on 23 August 2008.

Editor's note: see the Books column on page 29 for a description of "Evolving Methods for Macromolecular Crystallography - The Structural Path to the Understanding of the Mechanism of Action of CBRN Agents", edited by Randy Read and Joel Sussman, which came out in hardcover in June 2007, and in paperback in March, 2008. The final chapter in the book is a review by David Sayre titled Single Particle Imaging.

Douglas Rees, Robert Stroud and Jamie Cate to receive Protein Society Awards

The Protein Society announced its 2008 award recipients last November. The awards will be conferred at the 22nd Symposium to be held July 19-23, 2008 in San Diego, California.The **2008 Dorothy Crowfoot Hodgkin Award**, sponsored by Genentech, will be presented to **Douglas Rees,** Howard Hughes Medical Institute Investigator and Professor of Chemistry, Caltech, "for his fundamental contributions to the understanding of the structural biology of metalloproteins and membrane proteins, most notably by his analyses of the nitrogenase molybdenum-iron (MoFe-) protein that established the unprecedented structure of the FeMo-cofactor providing the active site for biological nitrogen fixation." His work also resulted in: the first structure determination of a physiologically gated ion channel, the mechanosensitive channel of large conductance (MscL) from *Mycobacterium tuberculosis*; and the first structure determination of an intact and fully ordered member of the widespread family of ABC transporters, the *E. coli* importer BtuCD for vitamin B12. (Solving the structure of vitamin B12 itself, many years ago, happens to be one of the main accomplishments of Dorothy Crowfoot Hodgkin.)

The **2008 Hans Neurath Award**, sponsored by the Hans Neurath Foundation, will be presented to **Robert Stroud**, UCSF Professor of Biochemistry, Biophysics, and Pharmaceutical Chemistry, "for his significant contributions to the understanding of structure function relationships in enzymes and membrane proteins." His work has focused on the molecular levels of cellular signaling and communication across cell membranes as well as the macromolecular encoding of specificity and affinity at protein/protein and protein/ligand interfaces. He has determined the high resolution three dimensional structures of numerous proteins of different classes and used these structures to define biological, biochemical, and cellular function - as templates for drug design. Stroud's seminal contribution of defining the mechanism of zymogen activation by demonstrating structurally that the catalytic site becomes rearranged is now taught in most undergraduate biochemistry courses. His recent studies on enzyme mechanism focus on thymidylate synthase with an emphasis on designing better drugs, and polyketide synthases with an emphasis on exploring biotechnological opportunities of producing new polyketide compounds. Another recent highlight includes the structure of the EPO-EPO receptor complex, which shows a 2:1 stoichiometry of binding for the cytokine and provides a major contribution to our understanding of cell surface signaling.



The **2008 Irving Sigal Young Investigator Award**, sponsored by Merck, will be presented to **Jamie Doudna Cate**, Professor of Chemistry, Biochemistry and Molecular Biology, UC Berkeley, "for his outstanding pioneering scientific contributions to the field of structural biology, particularly to our understanding of the structures of RNA and ribosomes." As a postdoctoral student, Cate solved the crystal structure of the entire 70S ribosome at 5.5 Å resolution, which at 2.5 MDaltons remains the largest asymmetric structure ever solved by x-ray crystallography. His research as an independent investigator has continued at the cutting edge of RNA and ribosome research, focusing on the *E. coli* ribosome. Last year, his group published a paper in *Science* describing the 3.5 Å structure of two conformational states of the *E. coli* 70S ribosome - the first all-atom structure of the complete ribosome.

New AAAS Fellows

Congratulations to **William L. Duax,** Hauptman-Woodward Medical Research Institute, **Janet L. Smith,** University of Michigan and **Thomas A. Steitz**, Yale University, who were elected AAAS fellows *because of their scientifically or socially distinguished efforts to advance science or its applications*. They were inducted at the Fellows Forum in February during the 2008 AAAS Annual Meeting in Boston.

Radu Custelcean Will Receive the 2008 Etter Award

As announced in the fall, 2007 issue of *ACA RefleXions*, the 2008 **Margaret C. Etter Early Career Award** will be presented to **Radu Custelcean**, Research Staff Member, Chemical Sciences Division, Oak Ridge National Laboratory at the ACA Annual Meeting in Knoxville, TN where he will give the keynote lecture at a symposium organized in his honor. Because the announcement was made just before the fall issue went to press, there was not enough space for the full citation, which follows.

Radu received his B.S. in chemistry in 1995 from Babes-Bolyai University in Romania; his M.S. in organic chemistry from that university the next year; and his Ph.D. in chemistry from Michigan State University in 2000. He was a postdoctoral associate in Mike Ward's lab at the University of Minnesota, and later in Yogendra Gupta's lab at the Institute for Shock Physics, Washington State University prior to his move to ORNL. His research has been featured on the covers of the *European Journal of Inorganic Chemistry* (2005), *ChemComm* (2005), and *Angewandte Chemie* (2005). His *ChemComm* paper also was headlined on the CAS webpage (January 23, 2006). He has been cited 533 times for his 30 papers listed in the Web of Science. (on 24 of which he is senior author). He has been a member of the ACS since 1998, and the ACA since 2005, and has served as a reviewer for many journals. In 2005, he was also among the top three Finalists for the Early Career Award for Scientific Accomplishment, UT-Battelle, and was selected by the Romanian newspaper *Cotidianul* to be among the top 33 young Romanian scientists.

Radu Custelcean is a rising star working in the exciting field of crystal engineering of hydrogen-bonded and coordination framework materials, e.g., metal-organic-frameworks (MOFs). These can be viewed truly as nanostructured materials, which are demonstrating utility for molecular recognition, separations chemistry, catalysis, and hydrogen storage. He routinely works on problems by designing new crystal architectures with desired functionality, growing the desired crystals, solving and refining the crystal structures using x-ray crystallography, and testing the chemical properties and functionality in models and important reactions. To give some examples of his research success, he designed a novel approach to anion separation that involves competitive crystallization of MOFs functionalized with hydrogen-bonding groups for specific anion coordination; he conceived a new strategy for controlling the assembly of molecular solids based on steric control over hydrogen bonding; he recognized and demonstrated that the simple meso-octamethylcalix[4]pyrole molecule possesses the remarkable ability to simultaneously host both a cation and anion in elegant solid state self-assemblies; and he demonstrated unprecedented encapsulation of sulfate by hydrogen bonding in a novel MOF. Radu is also working closely with theorists to provide feedback for computer aided molecular design methods. These methods offer opportunities for *de novo* structure-based design that, combined with high-throughput screening methods, can identify promising anion host architectures prior to synthesis and binding-affinity measurements. In 2003, at ORNL, Radu set-up an x-ray crystallography laboratory based on his purchase of a Bruker Diffractometer equipped with a CCD and a cryo-cooler. Rather than using this diffractometer in a service mode, Radu uses it as one of several tools in an integrated research program. His research is all hands-on, and he is a skilled experimentalist. Radu is becoming increasingly involved with the ACA, and organized a session at the 2005 meeting entitled "Microporous Metal-Organic Framework Solids." He has planned a related session on crystal engineering for the 2008 meeting in Knoxville. He sees crystal engineering as a topic which will be a mainstay at every ACA meeting for years to come. Classical crystal structure solution and refinement are at the heart of all of his research to date. Given the quality and quantity of his independent research at such a young age, we can expect Radu to have a long and distinguished career. His fields of interest are no accident. He recognizes the significance of crystal engineering beyond its current popularity, and is directing his efforts where the impact will be great. Radu's current position is a research scientist at a national laboratory, but I can easily envision him, later in his career, at a major university mentoring many students. It is fitting that his interests in crystal design using conventional and non-conventional hydrogen bonding align so well with those of Margaret Etter, who this award honors.

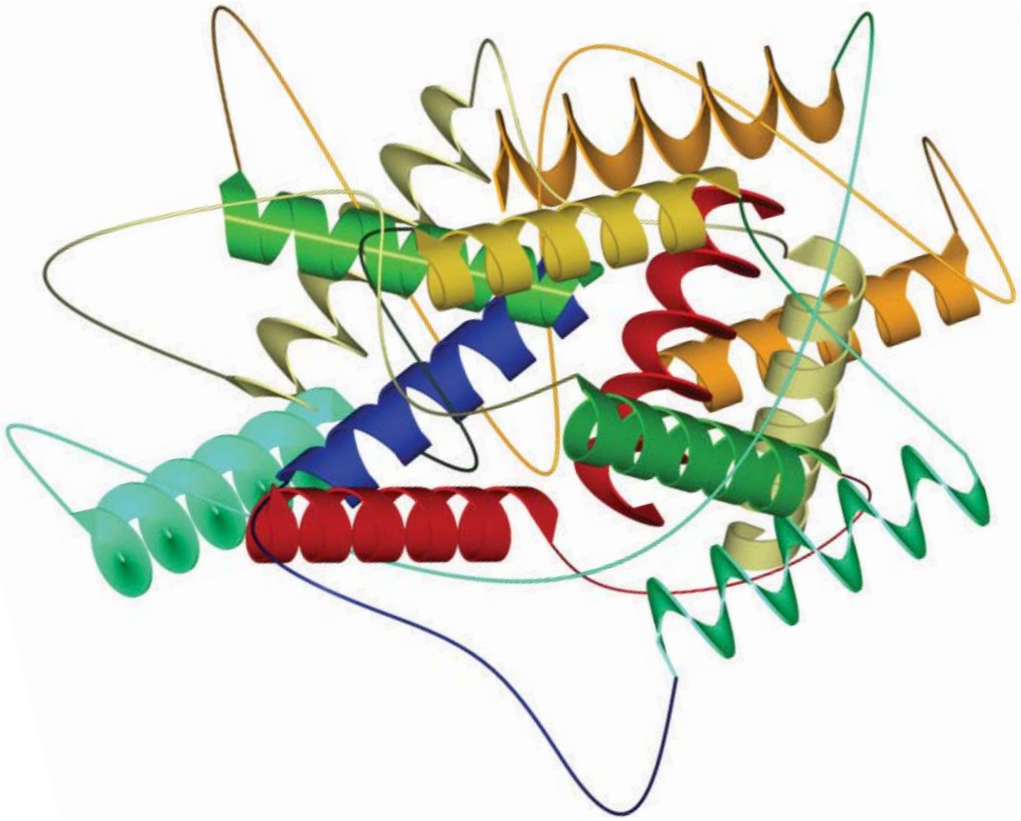
Bryan Chakoumakos

***Trillium grandiflorum* in spring, a Great Smoky Mountain photo from from nps.gov/grsm/photosmultimedia/index.htm**

2008 Bruker-AXS Scholarship

Again this year Bruker-AXS has chosen to recognize academic achievement by presenting a $6000 **Excellence in X-ray Diffraction** scholarship for the most unique application report in the areas of nanotechnology, materials science, geology or chemistry. Judging will be conducted by a panel of recognized experts in academia and industry. All application papers that are submitted become the property of Bruker -AXS and will be published in an annual volume, both in print and electronically. See the Bruker website **www.bruker-axs.com,** or contact Angie Grossen; tel: 608-276-3045, or 1-800-234-XRAY; **angie.grossen@bruker-axs.com** for more information.

High Throughput Dynamic Light Scattering



- High Sensitivity
- Low Sample Volume
- Temperature Control
- Automation Ready
- Your Choice of Microplates
  Compatible with SBS standard microplates. 96 & 384 well, clear, black, colored, strip wells, quartz... your choice, not ours.

The new Viscotek HorizonDLS™ is a state-of-the-art high throughput Dynamic Light Scattering instrument that generates the most sensitive and accurate performance available. It incorporates independent temperature control of the plate and the sample. Designed for use with a wide range of industry standard 96 or 384 well micro-plates, it delivers the same sensitivity, low sample volume, temperature control and performance as the acclaimed 802DLS™, but automatically, from the entire plate or selected wells, with no user intervention.

800-375-5966 **www.viscotek.com**

Viscotek™

a Malvern company

2008 Dues are Due

Please renew promptly and remember to support your favorite ACA Award Funds. NOTE: It is now possible to renew online at **www.AmerCrystalAssn.org.**

Congratulations to our staff photographer, Peter Müller and Claire Gallou-Müller on the birth of their daughter Ellen Gesine Marie!

Notes from the Editors

We are accepting entries to the **2009Art in Crystallography Contest** in the form of images emailed to either Editor (**conniechidester@earthlink.net** or **flippen@rcsb.rutgers.edu**). Entries should be accompanied by a paragraph explaining the science and the method of producing the image. A photo of the artist would be appreciated but is not required. Prizes consist of a small monetary award and a banquet ticket at the annual meeting. Winning entries will be posted on the web and will be displayed at the ACA Meeting. (Winners are not required to attend the meeting). We will also feature images in *ACA RefleXions* from time to time. Please let us know if you are interested in being a judge.

We are also seeking volunteers for a **Guest Editor** position. We're defining a guest editor as one who would be in charge of two or three pages in one issue of *RefleXions* on a specific subject: edit material solicited from others, assemble pictures, etc. Subjects might be, for example, Crystallography Education; Synchrotron Facilities; SAS & SASX; Nanoscience; PDF theory & techniques, -but other ideas would be welcome. We have lined up one volunteer already. For our winter issue, **Carrie Wilmot** has agreed to manage an article on Etter Award recipients - what the award has meant to them and what they are doing now.

Summer 2008 Travel Funds Available

Rigaku Americas Corporation will award summer travel bursaries (to be used for travel to a scientific conference) in the amount of $500 each to the five (5) post-doctoral fellows who provide the most compelling explanation as to how they intend to pursue a career in structural biology. Applications must be received by May 4, 2008 (**www.rigaku.com/protein/postdoc.html**).

The Pittsburgh Diffraction Society announces that it will make travel awards to outstanding graduate students who plan to attend and participate in the Osaka IUCr Congress. Applications for the awards, which are competitive, can be made at the Pittsburgh Diffraction Society website (**www.pittdifsoc.org**). Click on the link for the **George Jeffrey Award** and carefully follow the application instructions. The awards honor the memory of George A. Jeffrey, an influential crystallographer who believed strongly in promoting graduate studies in the diffraction sciences and in the importance of international cooperation.

ACA Council News

2008 ACA Meeting

The 2008 annual ACA meeting is approaching this spring, May 31 – June 5, in Knoxville, Tennessee. The proximity of Knoxville to Oak Ridge provides meeting attendees the opportunity to visit the newly constructed Spallation Neutron Source (SNS) at Oak Ridge National Laboratory - see page 31 for information. At this meeting, the Patterson Award will be presented to B.C. Wang. and the Margaret C. Etter Early Career Award will be presented to Radu Custelcean. Council looks forward to seeing everyone in Knoxville.

Meeting Abstracts: Books and CDs:

Council is transitioning to a CD distribution of the meeting abstracts. This move presents several advantages, including lower costs, later deadlines for abstract submission, fewer restrictions on abstract length, and easier archiving. The first phase of the transition will be evident at the upcoming ACA meeting in Knoxville.

Meeting attendees will be offered the choice of either the program and abstract book or the program schedule with abstracts on CD. For those who request both media, the second format will be available for a cost. New this year will be the availability on the ACA web site, prior to the meeting, of the complete Program & Abstract Book.

Picasso Meets Crystallography: A New Play

Cele Abad-Zapatero has written a one-act play, *Picasso Meets Crystallography*, based on the historical meeting between J.D. Bernal and Pablo Picasso on November 12, 1950. See page 27 for an account by Cele of the first reading of the play at the University of Illinois at Chicago last November. His play explores the relationship between the sciences and the arts and is scheduled to premier in early May at the Advanced Photon Source 2008 Annual Users Week Meeting. The filming of a documentary based on the development and production of the play will follow. ACA Council supports this project, with the intent that both the recorded premier production of the play and the documentary will be presented at a future ACA meeting.

Viscotek Acquired by Malvern Instruments

17 January 2008: Malvern, UK: materials characterization company Malvern Instruments, headquartered in Malvern, UK, has acquired Viscotek Corporation, a leading provider of chromatography solutions for the characterization of natural and synthetic polymers and proteins. Viscotek Corporation, headquartered in Houston, Texas, was founded in 1984 by Max Haney, inventor of the four-capillary differential viscometer detector. Viscotek's present management team will continue to lead the business, which will operate as Viscotek Corporation, a Malvern Company.

You've helped us with our research...

...now let us return the favor

With over 20 years experience in developing low temperature devices for X-ray crystallography, we've learnt a lot about our customers.

Keeping in close contact with the crystallographic community has allowed us to listen to your requirements and ideas, adapt our systems to suit and now enables us to offer a broad range of systems to cater for a variety of needs.

For instance, we have developed a wider range of temperatures with our Cryostream Plus and created the Cryostream Compact for optimal alignment with capillary powder samples in smaller enclosures. For those who prefer to use gaseous rather than liquid nitrogen, we have also introduced the Cobra non-liquid Cryostream.

In addition, our excellent reputation for technical support further explains why we are the preferred provider of variable temperature devices to the global crystallographic community.

For further information visit our website at www.oxcryo.com

OxfordCryosystems

Canadian News

There is a rookie reporter on the Canada beat and he needs your help. Send any interesting stories, event reports, workshop information, job postings, etc. to **britten@mcmaster.ca** and I'll pass them on. Also, the Canadian National Committee for Crystallography is compiling information for the *Crystallography in Canada* edition of the *IUCr Newsletter*. If you are willing to contribute articles on historical, current, or even future crystallographers or their accomplishments, please contact **Lachlan Cranswick** at **lachlan.cranswick@nrc.gc.ca**.

Toronto will be hosting the ACA meeting in 2009. We'll have some fun. The Buffalo office has most things organized as usual, and we'll start putting together a program in Tennessee. Those of you opting for Osaka instead of Knoxville, please contact me (**britten@mcmaster.ca**) or your favorite SIG chair if you have any session ideas. What about Canadian nominees for awards?

The Canadian Light Source Annual Users' Meeting will be held in Saskatoon, on June 9-10, 2008. The meeting is a great opportunity to learn about the progress of the Canadian Light Source, present your recent synchrotron work and meet fellow users. This years' meeting will be held in conjunction with the Fifth International Workshop on Mechanical Engineering Design of Synchrotron Radiation Equipment and Instrumentation (MEDSI) and the Fifteenth Pan-American Synchrotron Radiation Instrumentation (SRI) Conference, June 10-13, 2008. Joint workshops will be held on June 10. Watch for upcoming program and registration information at **www.lightsource.ca/uac/meeting2008/.**

The Third Saskatoon Synchrotron Summer School will take place August 18-22, 2008. The purpose of the school is to aid researchers who wish to add synchrotron techniques to their skill set. Information is presented through lectures, case studies, and practical hands-on experience, collecting and analyzing data. For more information, please go to **www.lightsource.ca/education/summerschool/.**

The Canadian Macromolecular Crystallography Facility, CMCF 08ID-1, is accepting proposals for beamline access during its commissioning stage. Pawel Grochulski submitted the following update:

Several improvements to the beamline were realized during the year 2007. The first MAD data collection at the Se-edge became possible after the small gap- in-vacuum undulator (SGU) was repaired allowing a 5.9 mm gap. Also efforts have been made to introduce automatic large energy changes. To this end a new Oxford BPM was installed in the end station and in collaboration with the CLS ring physicists a feed-forward procedure is being implemented to counteract orbit distortions and photon beam displacement from insertion device operation. Also, to protect the CCD detector, a light curtain was installed on the CCD holder. The cryo-jet nozzle was motorized to facilitate easy crystal mounting on the goniometer. A servo motor with a Parker controller was installed to improve shutter/goniometer synchronization. Fully functional graphical user interface and data collection software has been developed and implemented at the beamline. A script, autoxds, has been developed to facilitate full automation of the data processing with minimum intervention from a user. Other data processing software such as HKL2000 and CCP4 package are also available. The beamline is now equipped with a top of the line multi-core Dell server capable of running eight concurrent processes. This has greatly reduced the time required to process diffraction images and solve structures at the beamline.

For more details, contact Pawel at **Pawel.Grochulski@lightsource.ca**, 306-657-3538 or visit **www.lightsource.ca/cmcf.php.**

Planning for the Brockhouse Sector for Diffraction and Scattering is underway. The majority of the funding is in place to start the detailed design and construction of this materials characterization set of beamlines. **Stefan Kycia** (**stefan@physics.uoguelph.ca**) held a beamteam meeting in Toronto this winter to discuss the project, which in 2011 should provide access to simultaneous single crystal diffraction, high energy powder diffraction, and scattering experiments from both undulator and wiggler sources.

Neutron Diffraction plays an important role in the characterization of materials, and this is a year of transition in the US. People are very welcome to apply for neutron beamtime at the NRC facility in Chalk River, Ontario. The main crystallography instrument is the C2 neutron powder diffractor and beamtime proposals can be submitted at any time throughout the year. Information about the instrument is at **http://neutron.nrc-cnrc.gc.ca/c2gen_e.html** and queries can be sent to the C2 beamline scientists, **Ian Swainson** (**ian.swainson@nrc.gc.ca**) or **Lachlan Cranswick** (**lachlan.cranswick@nrc.gc.ca**).

Workshops on the northern horizon include the Alberta Powder Diffraction Workshop (**www.cins.ca/apdw/**) in Edmonton, scheduled for Wednesday 14th May 2008 to Friday 16th May 2008. The meeting will concentrate on Rietveld analysis using GSAS on the first two days, and then clay analysis using the BGMN Rietveld on the third day.

There has been talk of holding a short small molecule workshop for chemists, associated with the Canadian Society for Chemistry (CSC) meeting in Hamilton, ON, May 2009. Anyone interested in participating or helping out should contact Jim Britten (**britten@mcmaster.ca**).

On a sad note, Paul Michaud, formerly the Siemens Electric x-ray salesman for Canada, has passed away at the young age of 59. Those of you who knew Paul will remember his entertaining conversations about anything and everything. His character was never compromised by his job description.

Jim Britten

Great Smoky Mountains photo from nps.gov/grsm/photos-multimedia/index.htm

ACA COUNCIL OFFICERS - 2008

PRESIDENT

Marvin Hackert
Dept of Chem & Biochem
U Texas Austin
1 University Station A5300
Austin TX 78712
512 471 1105
Fax: 512 471 8696
m.hackert@mail.utexas.edu

VICE PRESIDENT

Robert (Bob) von Dreele
IPNS Div
Argonne Nat'l Lab
Argonne, IL 60439
630 252 8178
Fax: 630 252 4163
vondreele@anl.gov

PAST PRESIDENT

A. Alan Pinkerton
Dept. of Chemistry
U Toledo
2801 W. Bancroft St.
Toledo, OH
43606-3390
419-530-4580
apinker@uoft02.utoledo.edu

TREASURER

Bernie Santarsiero
M/C-870
Ctr For Pharm Biotech
U Illinois Chicago
3100-MBRB
900 S Ashland Ave
Chicago IL 60607
312 413 0339; Fax: 312 413 9304
bds@uic.edu

SECRETARY

Lisa J. Keefe
IMCA-CAT,
Sector 17,
Bldg. #435A
Advanced Photon Source
Argonne Nat'l Lab
9700 South Cass Ave.
Argonne, IL 60439
630-252-0544; Fax: 630-252-0521
keefe@anl.gov

CANADIAN REPRESENTATIVE

James F Britten
Dept of Chem ABB-417
McMaster U
1280 Main St W
Hamilton Ontario
Canada, L8S 4M1
905-525-9140 ext 23481
Fax: 905-522-2509
britten@mcmaster.ca

APPOINTMENTS

CHIEF FINANCIAL OFFICER

S.N. Rao,
Max Chambers Library Room 221
U Central Oklahoma
100 N. University Dr.
Edmond, OK 73034-5209
405-974-2524
Fax 405-974-3852
srao@ucok.edu

CHIEF EXECUTIVE OFFICER

William L. Duax
Hauptman Woodward Medical Res. Inst.
700 Ellicott St.
Buffalo, NY 14203-1196
716-898-8616
Fax: 716-898-8695
duax@hwi.buffalo.edu

IUCr REPRESENTATIVE

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

EDITORS, *ACA RefleXions*

Judith Flippen-Anderson
3521 Launcelot Way
Annandale, VA 22003
703-346-2441
Fax: 716-898-8695
flippen@rscb.rutgers.edu

Connie Rajnak
4210 Old Field Trail
Kalamazoo, MI 49008
269-342-1600
Fax: 716-898-8695
conniechidester@earthlink.net

***RefleXions* STAFF PHOTOGRAPHER**
Peter Müller
(see address in Standing Committee listing, next page)

Editor's note: See page 7!

DIRECTOR OF ADMINISTRATIVE SERVICES

Marcia Colquhoun
ACA, P.O. 96 Ellicott Station
Buffalo, NY 14205-0096
716-898-8692; Fax: 716-898-8695
marcia@hwi.buffalo.edu

CANADIAN DIVISION

David Rose, *Chair*
Ontario Cancer Institute
U Toronto, Toronto, Ont.
Canada, M5G 2M9
416-946-2970
Fax: 416-946-6529

Pawel Grochulski, *Secretary*
Canadian Light Source
U Saskatchewan
101 Perimeter Rd
Saskatoon,
Saskatchewan
Canada, S7N 0X4
306-657-3538
Fax: 306-657-3535
pawel.grochulski@lightsourceca

Communications

Annie Heroux, Chair (05-08)
Dept. of Biology
Brookhaven National Lab
Bldg. 463 5000
Upton NY 11973
631-344-4454; Fax: 631-344-2741
heroux@bnl.gov

William T. Pennington (06-09)
Dept of Chemistry
Clemson Univ.
Clemson SC 29634
864-656-4200; Fax: 864-656-6613
billp@clemson.edu

Alice Vrielink (07-10)
Dept Of Chem & Biochem
Univ Of California Santa Cruz
1156 High St
Santa Cruz CA 95064
831 459 5126; Fax: 831 459 3139
vrielink@biology.ucsc.edu

Allen Oliver (08-11)
Chemistry & Biochemistry
Univ. of California Santa Cruz
1156 High St
Santa Cruz CA 95064
831 459 2892
aoliver@chemistry.ucsc.edu

Continuing Education

Gloria Borgstahl, Chair (05-08)
The Eppley Inst For Cancer Research
987696 Nebraska Med. Ctr.
Omaha, NE 68198-7696
402-559-8578;
Fax: 402-559-8577
gborgstahl@unmc.edu

Christopher L. Cahill (06-09)
Dept of Chemistry
George Washington Univ
725 21st St NW
Washington DC 20052
202-994-6959; Fax: 202-994-5873
cahill@gwu.edu

William Furey (07-10)
Dept of Pharmacology
Univ of Pittsburgh
Lothrop St.
Pittsburgh PA 15261
Fax: 412 688 6945
fureyw@pitt.edu

Peter Müller (08-11)
Dept. of Chemistry Bldg 2 Rm 325
MIT
77 Massachusetts Ave
Cambridge MA 02139
617 253-1884
pmueller@mit.edu

Data, Standards & Computing

Bernhard Rupp, Chair (05-08)
Q E D Life Science Discovery
6487 Half Dome Ct
Livermore, CA 94551
925-209-7429; Fax: 801-880-3982
bernhardrupp@sbcglobal.net

Andy Howard (06-09)
Biol. Chem. & Phys. Science
Illinois Inst of Tech
3101 S Dearborn
Chicago IL 60616
312-567-5881; Fax: 312-567-3576
howard@iit.edu

Winnie Wong-Ng (07-10)
Mat Science & Eng Lab
NIST
Bldg 223 Rm A256
Gaithersburg MD 20899
301 975 5791; Fax: 301 975 5334
winnie.wong-ng@nist.gov

David Harrison (08-11)
Biochemistry & Molecular Biology
Rosiland Franklin Univ. of Medicine
& Science
3333 Green Bay Rd
Chicago IL 60064
847 578 8609; Fax: 847 578 3240
david.harrison@rosilandfranklin.edu

SPECIAL INTEREST GROUP OFFICERS 2008

Biological Macromolecules

Carrie Wilmot, Chair, 08
Dept of Biochem Mol Bio & Biophys
6-155 Jackson Hall 321 Church St SE
Univ of Minnesota
Minneapolis, MN 55455-0326
612 624 2406; Fax: 612 624 5121
wilmo004@umn.edu

John Horton, Chair Elect 08
Dept. of Biochem
Emory Univ.
1510 Clifton Rd
Atlanta GA 30322
404 727 8492
jrhorto@emory.edu

John Tanner, Sec./Treas., 07-08
Dept of Chemistry
Univ of Missouri Columbia
125 Chemistry Bldg
Columbia MO 65211
573 884 1280; Fax: 573 882 2754
tannerjj@missouri.edu

Fiber Diffraction

Joseph Orgel, Chair, 08
Dept BCPS
Illinois Inst.Technology
3101 S Dearborn
Chicago, IL 60616
312 567 3398; Fax: 312 567 3494
orgel@iit.edu

Gerald Stubbs, Past Chair, 08
Biological Sciences
Vanderbilt Univ.
VU Station B Box 35-1634
Nashville, TN 37235-1820
615 322 2018; Fax: 615 343 6707
gerald.stubbs@vanderbilt.edu

Amy Kendall, Secretary, 08
Biological Sciences
Vanderbilt Univ.
VU Station B Box 35-1634
Nashville TN 37332
615 322-2012; Fax: 615 343 6707
amy.k.kendall@vanderbilt.edu

General Interest

Allen Oliver, Chair, 08
Dept of Chemistry
Univ of California Santa Cruz
1156 High St
Santa Cruz CA 95064
831 459 2892
aoliver@chemistry.ucsc.edu

Bruce C. Noll, Chair-elect 08
Chemistry & Biochemistry
260B Nieuwland Science
Univ. of Notre Dame
Notre Dame IN 46556
574 631 5935; Fax: 574 613 6652
bnoll@nd.edu

Jeanette Krause, Sec./Treas., 08
Dept of Chemistry
Univ. of Cincinnati
Cincinnati OH 45221-0172
513 300 3296; Fax: 513 556 9239
jeanette.krause@uc.edu

Nathan Coker, Member at Large, 08
Dept of Physics Science
Morehead State Univ
425B Lappin Hall
Morehead KY 40351
606 783 2910; Fax: 606 783 5002
nl.coker@morehead-st.edu

Industrial

Herbet Klei, Chair, 08
Bristol-Myers Squibb
Pharm Res Inst
PO Box 4000 (H23-06)
Princeton NJ 08543-4000
609 252 4359
herbert.klei@bms.com

Susan Byram, Secretary, 08
Bruker AXS Inc
5465 E Cheryl Pkwy
Madison WI 53711
608 276 3041; Fax: 608 276 3006
sue.byram@bruker-axs.com

Materials Science

Branton Campbell, Chair, 08
Dept of Physics & Astronomy
Brigham Young Univ
N261 ESC BYU
Provo UT 84602
801 422 5758
branton_campbell@byu.edu

Pamela Whitfield, Chair-elect 08,
ICPET
National Research Council of Canada
Ottawa ON K1A 0R6 Canada
613 998 8462; Fax: 613 991 2384
pamela.whitfield@nrc.gc.ca

Claudia Rawn, Past Chair, 08
Oak Ridge National Lab
Metals & Ceramics Div
PO Box 2008 MS 6064
Oak Ridge, TN 37831
865 574 3184; Fax: 865 574 3940
rawncj@ornl.gov

Neutron Scattering

Ian Swainson, Chair 07
Canadian Neutron Beam Centre
Chalk River Labs
Chalk River ON
Canada K0J 1J0
613 584 8811 ext 3995
Fax: 613 584 4040
ian.swainson@nrc.ca

Thomas Proffen, Chair-elect 08
Neutron Scattering Center
Los Alamos National Lab
LANSCE-12 MS H805
Los Alamos NM 87545
Tel: 505 665 6572
Fax: 505 665 2676
tproffen@lanl.gov

Paul Langan, Past Chair 08
Dept. of Bio. Sci., M888
Los Alamos National Laboratory
Los Alamos, NM 87545
505 665 8125; Fax: 505 665 3025
langan_paul@lanl.gov

Powder Diffraction

Cora Lind, Chair, 08
Dept. of Chemistry MS 602
Univ. of Toledo
Toledo OH 43606
419 530 1505; Fax: 419 530 4033
cora.lind@utoledo.edu

Ashfia Huq, Chair-elect 08
Neutron Scattering Science Div
Spallation Neutron Source
Oak Ridge National Lab
PO Box 2008 MS 6475
Oak Ridge TN 37831
865 574 7923
huqa@ornl.gov

Thomas Proffen, Past Chair, 08
Los Alamos National Laboratory
Manuel Lujan Jr Neutron Scat. Ctr.
LANSCE-12, MS H805
Los Alamos, NM 87545
505 665 6573; Fax: 505 665 2676
tproffen@lanl.gov

Service Crystallography

Peter Müller, Chair 08
Dept of Chemistry, MIT
Bldg 2 Rm 325
77 Massachusetts Ave
Cambridge MA 02139
pmueller@mit.edu

Dale Swenson, Chair-elect 08
Dept. of Chemistry
Univ. of Iowa
Iowa City IA 52242
319 335 0291; Fax: 319 335 1270
dale-swenson@uiowa.edu

Bruce Noll, Secretary, 08
Chemistry & Biochemistry
260B Nieuwland Science
Univ. of Notre Dame
Notre Dame IN 46556
574 631 5935; Fax: 574 613 6652
bnoll@nd.edu

Small Angle Scattering

P. Thiyagarajan, Chair, 08
IPNS Bldg 360
Argonne Nat'l Lab
9700 S Cass Ave
Argonne IL 60439
630 252 3593; Fax: 630 252 4163
thiyaga@anl.gov

Kenneth Littrell, Chair elect 08
CG2 SANS Instrument Scientist
Neutron Scattering Sci Div/High Flux Isotope Reactor
Oak Ridge National Laboratory
One Bethel Valley Road
Oak Ridge, TN, 37831-6393 USA
865 574-4535
littrellkc@ornl.gov

Thomas Weiss, Sec/Treas. '08
SSRL/SLAC
Stanford Univ.
2575 Sand Hill Rd MS69
Menlo Park CA 94025
650 926 4078; Fax: 650 926 4100
weiss@slac.stanford.edu

Alec Sandy, Member at Large, 08
Advanced Photon Source
Argonne National Lab
9700 S Cass Ave
Argonne IL 60439
630 252 0281; Fax: 630 252 0282
asandy@aps.anl.gov

Small Molecules

Kraig Wheeler, Chair, 08
Dept of Chemistry
Eastern Illinois Univ
600 Lincoln Ave
Charleston IL 61920-3099
217 581 3119
kawheeler@eiu.edu

Jeanette Krause, Chair-elect., 08
Dept of Chemistry
Univ. of Cincinnati
Cincinnati OH 45221-0172
513 300 3296; Fax: 513 556 9239
jeanette.krause@uc.edu

Allen Oliver, Sec/Treas, 08
Chemistry & Biochemistry
Univ. of California Santa Cruz
1156 High St
Santa Cruz CA 95064
831 459 2892
aoliver@chemistry.ucsc.edu

Synchrotron Radiation

Richard Gillilan, Chair, 08
MAC CHESS
Cornell Univ
200L Wilson Lab
Ithaca NY 14853
607 255 9386
reg8@cornell.edu

Ernst Bergmann, Chair-elect 08,
Alberta Synchrotron Inst.
Res Transition Facility Suite 2080
Univ. of Alberta
Edmonton AB T6G 2E1 Canada
780 492 8249; Fax: 780 492 6160
ernst.bergmann@ualberta.ca

James Holton, Past Chair, 08
Lawrence Berkeley Nat'l Lab
Dept Of Biochem & Biophys
1 Cyclotron Rd
Berkeley, CA 94107
510 486 4587; Fax: 510 486 5298
jmholton@lbl.gov

Young Scientists

Peter Horanyi, Chair, 08
Mol Physiol & Biol. Physics
Univ. of Virgina
1340 Jefferson Park Ave
Charlottesville VA 22908
706 461 0534
magyar@virginia.edu

Bobby Huether, Chair-elect 08,
Hauptman Woodward MRI
700 Ellicott St
Buffalo NY 14203
716 898 8678; Fax: 716 898 8660
bhuether@hwi.buffalo.edu

Mark Collins, Secretary, 08
Dept of Biochem & Mol Biophys
Columbia Univ
630 W 168th St
New York NY 10032
212 304 3456
MNC2003@columbia.edu

2008 U.S. NATIONAL COMMITTEE FOR CRYSTALLOGRAPHY

Chair

JAMES A. KADUK (08)

INEOS Technologies
150 W. Warrenville Road
P.O. Box 3011, MC F-9
Naperville, IL 60566
630-420-4547
Fax: 630-420-5252
james.kaduk@innovene.com

Vice-Chair

KATHERINE KANTARDJIEFF (08)

Dept. of Chem. & Biochem.
California State U., Fullerton
800 N. State College
Fullerton, CA
92834-9480
714-278-3752
Fax: 714-278-5293
kkantardjieff@fullerton.edu

Secretary-Treasurer

DOUGLAS OHLENDORF (09)

Dept. Biochem., Mol. Biol. & Biophys.
6-155 Jackson Hall
Univ. of Minnesota
321 Church St. S.E.
Minneapolis, MN 55455
612-624-8436
Fax: 612-624-5121
ohlen@umn.edu

Members

CHRISTOPHER CAHILL (09)

George Washington Univ.
Dept. Chemistry
725 21st Street NW
Washington, DC 20052
202 994 6959
Fax: 202 994 5873
cahill@gwu.edu

JULIA Y. CHAN (10)

Louisiana State Univ.
Dept. Chem.
232 Chopin Hall
Baton Rouge, LA 70803
225-578-2695 / 5380
Fax: 225-578-3458
jchan@lsu.edu

CORA LIND (09)

Chemistry Dept.
2262 WO
Univ. Toledo
Toledo, OH 43606
419-530-1505
Fax: 419-530-4033
cora.lind@utoledo.edu

JOSEPH NG (09)

Dept. Biol. Science
Biol.Science WH 254
U.Alabama-Huntsville
Huntsville, AL 35899
256-824-3715
ngj@email.uah.edu

MIRIAM ROSSI (10

Vassar College
Dept. of Chemistry
124 Raymond Avenue
Poughkeepsie, NY 12601
484-437-5746; Fax: 484-437-5732
rossi@vassar.edu

BERNHARD RUPP (10)

Q.E.D. Life Sci. Discoveries, Inc.
6487 Half Dome Court
Livermore, CA 94551
955-209-7429
br@qedlife.com

STEVEN SHERIFF (10)

Research Fellow
Bristol Myers-Squibb
Dept.Macromolec.Struc.
P.O. Box 5400
Princeton, NJ 08543
609-252-5934
steven.sheriff@bms.com

CHERYL L. KLEIN STEVENS (08)

Dept. of Chemistry
Xavier Univ. of Louisiana
1 Drexel Drive
New Orleans, LA 70125
504-483-7377;
Fax: 504-485-7942
cklein@xula.edu

JENNIFER SWIFT (08)

Dept. of Chem.
Georgetown Univ.
647 Reiss,
37th & O Streets NW
Washington, DC 20057
202-687-5567
Fax: 202-687-6209
jas2@georgetown.edu

BRIAN H. TOBY (09)

Argonne Nat'l Lab.,
APS
9700 S. Cass Ave
Bldg. 433/D003
Argonne, IL 60439-4856
630 252-5488
Brian.Toby@ANL.gov

ROBERT VON DREELE (09)

Argonne Nat'l Lab.
9700 S. Cass Ave
360/C-213
Argonne, Il 60439
630-252-8178
Fax: 630-252-5391
vondreele@anl.gov

VICTOR G. YOUNG JR. (08)

Dept. of Chemistry
Univ. of Minnesota
160 Kolthoff Hall
207 Pleasant Street S.E.
Minneapolis, MN 55455, USA
612 625-6897; Fax: 612 626-7541
young@chemsun.chem.umn.edu

Ex-Officio Voting Members

See ACA Officers Roster for addresses.

WILLIAM DUAX
IUCr Past-President

MARVIN HACKERT
ACA President

BERNARD D. SANTARSIERO)
ACA Treasurer

ROBERT VON DREELE
ACA Vice-President (photo above)

rayonix mx series

Seamless multi-element CCD X-ray detectors

mx225 **9 CCDs; 3k × 3k readout in 1 sec.**

mx300/mx325 **16 CCDs; 4k × 4k readout in 1 sec.**

- Low noise
- Lowest achievable dark current

Options:

- Ultrastable background for SAXS/WAXS
- Custom taper ratios
- Custom phosphor options

HE **High Efficiency models available**

High electro-optical gain design

The single CCD design **sx165** also offers the frame shift option to facilitate consecutive exposures only miliseconds apart in time.

rayonix

High-performance X-ray technology

www.rayonix.com

1880 Oak Avenue
Evanston, IL 60201 USA
info@rayonix.com

Tel: +1 (847) 869-1548
Fax: +1 (847) 869-1587
Toll Free in USA: (877) 627-XRAY

Subcommittee on Interdisciplinary Activities (non-voting members)

SCOTT MISTURE (08)
ICDD Representative
Alfred Univ.
misture@alfred.edu

PETER VEKILOV (09)
American Assoc. for Crystal Growth
Univ. of Houston
vekilov@uh.edu

PAUL VOYLES (09)
Microscopy Society of America
Univ. of Wisconsin
voyles@engr.wisc.edu

Ex-Officio Non-Voting Members

Gary Calabrese
(NAS) BCST Co-Chair
Rohm & Haas Company
215-592-3000
gcalabrese@rohmhaas.com

F. Fleming Crim
(NAS) BCST Co-Chair
University of Wisconsin
608-263-7364
fcrim@chem.wisc.edu

Michael Clegg,
NAS Foreign Secretary
Univ. California at Irvine
949-824-4490
mclegg@uci.edu

Kathie Bailey Mathae
Senior Program Officer
The National Academies
202 334 2606
kbmathae@nas.edu

Katie Bowman
Staff Officer, NAS
202-334-2638
kbowman@nas.edu

Pam Gamble
Admin. Assistant, NAS
202-334-2688
pgamble@nas.edu

The ACA Summer Course in Small Molecule Crystallography, 2008

The 10-day intensive course is tentatively scheduled for July 7 - 16, 2008 at the Indiana University of Pennsylvania. IUP is located in the town of Indiana about 80 miles east of Pittsburgh, PA. The course will cover both single crystal and powder diffraction and each day will consist of lectures in the morning, hands-on workshops in the afternoon and computer tutorials at night. While some advanced topics will be introduced (structure solution from powder data, advanced probability methods, solving difficult structures), the curriculum will mostly emphasize fundamental crystallography and no prior crystallographic experience will be assumed. Attendees are encouraged to bring their own single crystal or powder samples for x-ray data collection and are expected to have completed at least undergraduate courses in chemistry, physics and mathematics. They are advised to read in advance *Crystal Structure Analysis: A Primer*, by Jenny P. Glusker and Kenneth N. Trueblood, Oxford Univ. Press (1985).

The organizers aim for a total of 24 attendees, who in past years have come from the U.S. and abroad; from academia (students and faculty), from government and from corporations. There will be at least 12 experienced teaching faculty present. Tuition will be $250 (or $750 for applicants from corporate labs). Student apartment housing at IUP (including breakfast and lunch) is available for an additional $400 ($650 or $1,150 for corporate labs). Approximately 12 student scholarships will be offered (exceptional undergraduate students will be considered) and will consist of a waiver of tuition and living costs. The scholarships will be awarded based on: (1) scientific ability, (2) expected benefits from the course and (3) skills in English. We encourage applications from Latin America.

Instruments at IUP will include two Bruker-Nonius CAD4 single crystal diffractometers, a Bruker D8 Advance and a Rigaku Miniflex powder diffractometer. In the past three years, Rigaku-Americas brought a SCXmini X-ray Crystallographic System to the IUP laboratory. Students will also have access to the Duquesne University X-ray Facility which has a Bruker APEX II single crystal diffractometer and a PANalytical X'Pert Pro powder diffractometer. The IUP computer facilities are excellent and each student will have access to an individual computer during the nightly tutorials. Access will also be available to the Cambridge Structural Database and the ICDD powder diffraction database. The software used in the course will be Bruker-Nonius SHELXTL, Rigaku Americas CrystalClear, GSAS/EXPGUI, FullProf, CRYSFIRE and CRYSTMOL.

The Course registration form can be obtained from the ACA web site at **www.AmerCrystalAssn.org**. Completed forms must be received before May 26th, 2008 by Charles H. Lake, Chemistry Department, Indiana University of Pennsylvania, Indiana, PA 15705, USA or electronically at **lake@iup.edu** for full consideration. Further information will be updated on the web site or can be obtained from **lake@iup.edu** or **craven@icubed.com.**

We shall observe the basic policy of nondiscrimination and affirm the rights of scientists throughout the world to adhere or to associate with international scientific activity without restrictions based on nationality, race, color, age, religion, political philosophy, ethnic origin, citizenship, language, or sex, in accordance with the statutes of the International Council of Scientific Unions. At this Course, no barriers will exist which would prevent the participation of *bona fide* scientists. Foreign students may be accepted early to provide extra time to process Visa's.

Charles H. Lake and Bryan M. Craven, Organizers

My system is:

Rigaku

Leading With Innovation

At the forefront of X-ray technology

Generators

FR-E+ SuperBright™, MicroMax™-007 HF
MicroMax-002+

Detectors

R-AXIS IV++ dual IP, R-AXIS HTC triple IP
Saturn 944+ CCD

Optics

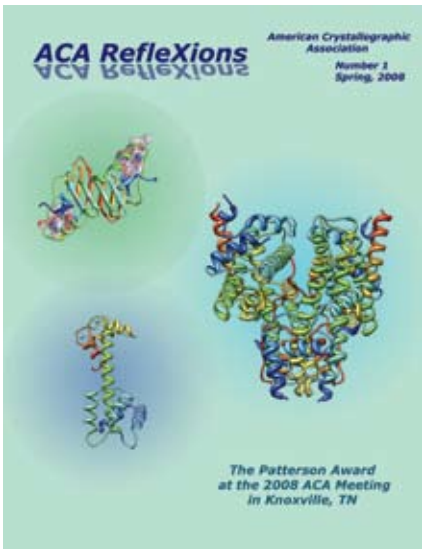
VariMax™ HF, VariMax HR, VariMax Cr

VariMax: Patent pending

www.Rigaku.com

Rigaku

Rigaku Americas Corporation phone: 281-362-2300 e-mail: info@Rigaku.com
Rigaku Europe phone: +[44] 1732 763367



On the Cover:

At the 2008 ACA Meeting in Knoxville the **A. Lindo Patterson Award** will be presented to **Bi-Cheng (B.C.) Wang**, Professor, Dept. of Biochemistry and Molecular Biology and Ramsey/Georgia Research Alliance Eminent Scholar in Structural Biology at the University of Georgia. The images on the cover were selected from many that have special significance to B.C.

At left, top: neurophysin, a hormone carrier protein, in complex with a dipepide. This was the first *de novo* structure solved from SAD data from an incorporated iodine atom using Wang's ISAS solvent flattening program. The asymmetric unit is an elongated tetramer of dimensions 110 x 40 x 30 Å, composed of two dimers related by pseudo twofold symmetry. Each monomer consists of two homologous layers, each with four antiparallel ß-strands. The two regions are connected by a helix followed by a long loop. Monomer-monomer contacts involve antiparallel ß-sheet interactions, which form a dimer with two layers of eight ß-strands. One peptide per monomer occupies the principal hormone-binding pocket formed by part of the amino-terminal region and parts of the connecting helix and loop, with binding to protein consistent with conclusions drawn from solution studies. Dimer-dimer contacts involve the Tyr49 region adjacent to this site. A fifth dipeptide, of unknown biological significance, helps to stabilize one of the monomer-monomer interfaces and the tetramer-tetramer network in the crystal. The image is from *Crystal Structure of a Bovine Neurophysin II Dipeptide Complex at 2.8 Å Determined from the Single-Wavelength Anomalous Scattering Signal of an Incorporated Iodine Atom*, L. Chen, J.P. Rose, E Breslow, D. Yang, W. Chang, W.F. Furey Jr, M. Sax and B.C. Wang, *PNAS USA*, 1991, **88**, 4240-4244. © 1991 by National Academy of Sciences.

At right: **The nucleosomal core (H2A-H2B-H3-H4)$_2$ histone octamer**. This was solved from SIR data using the ISIR solvent flattening program in collaboration with Moudruanakis and colleagues. The histone octamer is a tripartite assembly in which a centrally located (H3-H4)$_2$ tetramer is flanked by two H2A-H2B dimers. It has a complex outer surface; depending on the perspective the structure appears as a wedge or as a flat disk with diameter 65Å and length 60Å at its maximum and ≈ 10Å at the minimum. The histone octamer has regularly spaced ridges and valleys that define a left-handed protein superhelix with ≈28Å pitch, very suggestive of the path of the DNA superhelix in the nucleosome. *The nucleosomal core histone octamer at 3.1 A resolution: A tripartite protein assembly and a left-handed superhelix*, G. Arents, R.W. Burlingame, B.C. Wang, W.E. Love, and E.N. Moudrianakis, *PNAS*, **88**, 10148-10152, (1991).

At left, bottom: troponin C, which was solved from SIR data using B.C.'s ISIR solvent flattening program in collaboration with M. Sundaralingam and colleagues. The structure of troponin C (TnC), the Ca^{2+}-binding subunit of the troponin complex, shows that the protein is about 70 Å long with an unusual dumbbell shape. The carboxyl and amino domains are separated by a single long alpha helix of about nine turns. Only the two high-affinity Ca^{2+}-Mg^{2+} sites of the COOH-domain are occupied by metal ions resulting in conformational differences between the COOH- and NH_2-domains. These differences are probably important in the triggering of muscle contraction by TnC. The structure is relevant in understanding the function of other calcium-regulated proteins, in particular calmodulin because of its strong similarity in amino acid sequence. *Molecular Structure of Troponin C from Chicken Skeletal Muscle at 3Å Resolution*. M. Sundaralingam, R. Bergstrom, G. M. Strasburg, S. T. Rao, P. Roychowdhury, M. L. Greaser and B. C. Wang, *Science* **227**, 945-948 (1985).

We gratefully acknowledge the continued support of ACA CORPORATE MEMBERS and welcome new members

Active Sight
www.active-sight.com

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

Art Robbins Instruments
www.artrobbinstruments.com

ATPS Inc.
www.atpsinc.com

Axygen Biosciences
www.axygenbio.com

Bibliothek Technische Hochschule
Hannover, Germany

Biblioteca Universitaria
Oviedo, Spain

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

Bruker/AXS
www.bruker-axs.com

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

Charles Supper Company, Inc.
www.charles-supper.com

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

Crystal Logic Inc.
www.xtallogic.com

CyBio, Inc.
www.cybio-ag.com

Douglas Instruments Limited
www.douglas.co.uk

Emerald Biosystems
www.emeraldbiostructures.com

Fluidigm Corp.
www.fluidigm.com

Formulatrix
www.formulatrix.com

Hampton Research
www.hamptonresearch.com

Incoatec GmbH
www.incoatec.de

Jena Bioscience GmbH
www.jenabioscience.com

Korima, Inc.
www.korimainc.com

MiTeGen LLC
www.mitegen.com

Molecular Dimensions, Inc.
www.moleculardimensions.com

Neuro Probe, Inc.
www.neuroprobe.com

Oxford Cryosystems
www.oxfordcryosystems.com

Oxford Diffraction Ltd.
www.oxford-diffraction.com

Rayonix/MAR USA
www.mar-usa.com

RCSB-Protein Data Bank
www.rcsb.org/pdb

Rigaku Americas, Inc.
www.Rigaku.com

Thermo Fisher Scientific
www.thermo.com

TTP Labtech
www.ttplabtech.com

Viscotek Corporation
www.viscotek.com

Wyatt Technology
www.wyatt.com

Xenocs **SA**
www.xenocs.com

We are especially grateful to our Corporate Sponsors of the 2008 ACA Meeting

QUARTZ
Pulse Ray

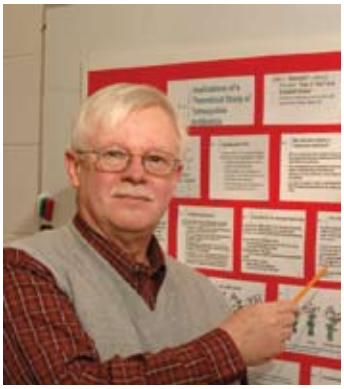
EMERALD
Hoffmann-La Roche Inc.
Pfizer Global R&D

RUBY

DIAMOND

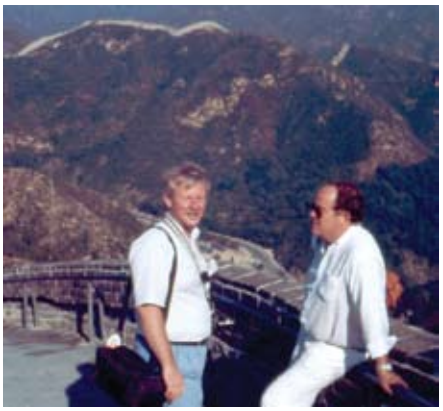
Area Detector Systems Corp
Hampton Research Corp
Merck Research Laboratories
Bruker AXS
International Union of Crystallography

John J. Stezowski 1942-2007



The crystallographic community lost a great leader, outstanding scientist, and one of its most engaging personalities with the untimely passing of John J. Stezowski. John was a Professor of Chemistry at the University of Nebraska-Lincoln at the time of his death, November 30, 2007.

John received his B.S. in Chemistry from Case Institute of Technology in 1964 and subsequently joined the research group of Prof. Harry Eick at Michigan State University where he engaged in a physical-inorganic chemistry project studying organometallic complexes. It was during this time that he displayed an affinity for the disciplines that would become his lifelong pursuits: chemistry education (he received a DuPont teaching fellowship in 1967) and crystallography. John often told his trainees that part of his thesis project involved determining a crystal structure, and from then on he was hooked. Upon receiving his Ph.D. in Chemistry in 1969, John moved on to conduct more crystallographic studies as an NIH Postdoctoral Fellow at Cornell University in the laboratory of Professor Lynn Hoard, and remained on staff as an Assistant Professor until 1972. He then assumed a position as a Wissenschflicher Assistant at the University of Stuttgart, later becoming Privatdozent and, in 1986, University Professor. While at Stuttgart, John established an internationally recognized crystallography program studying organometallic and bi-molecular organic complexes, cyclic peptides, and cyclodextrins. He was a champion of international crystallography and regularly presented at workshops in Poland and Hungary. One of the more "memorable" workshops in Poland concluded with John and Wolfram Saenger being challenged to leap over the celebratory bonfire. John accepted the challenge, leapt the fire, and broke his leg. He also spent a number of summers as a sabbatical scientist at Fox Chase Cancer Center in Jenny Glusker's group where he studied metalloproteins. He was an active leader in the crystallographic community. In 1984 he established, with assistance from Judith Flippen-Anderson and Bill Duax, the IUCr Commission on Small Molecules (known today as the Commission on Structural Chemistry), and served as its first chair. A particularly significant moment in international crystallography occurred in 1986 when John led a group to organize a special IUCr symposium in Beijing. The Chinese delegation had just lost out on a bid to host the 1990 IUCr meeting, so John approached them about the possibility of hosting a special IUCr symposium. The conference featured plenary lectures by Dorothy Hodgkin, Bill Lipscomb, Herb Hauptman and Jack Dunitz per John's request, and was a great success. In 1991, he took an appointment as Professor of Chemistry at the University of Nebraska-Lincoln where he built a research program focusing on chemical and protein crystallography, while also pouring much time and effort into enhancing undergraduate chemical education both in the classroom and through research experience in his lab. John authored more than 160 papers during his career and edited a number of symposia transactions on chemical crystallography and protein crystallization. His commitment to education continued undiminished to his final days, as he was working on a CD-ROM-based textbook on crystal structure determination at the time of his passing.



John with Peter Speh visiting the Great Wall during the Beijing meeting

John at the 1986 IUCr Symposium in Beijing. In the background can be seen (right to left) Herb Hauptman, Bill Lipscomb, and Dorothy Hodgkin (mostly occluded by someone's elbow).

To all those that knew him, John was the ultimate scholar, educator and researcher, but it was John's personality that we will remember and miss most of all. The crystallographic community has lost a valued member and a dear friend. In the weeks following his unexpected death, I was honored to hear from many current and former colleagues, trainees and students, who recounted with me their favorite stories of John. Outside of his scientific accomplishments he was well regarded as an excellent cook and enjoyed sharing his talents with his trainees and colleagues. His impact on the crystallography and chemistry communities through his generosity, mentorship and teaching is crystal clear.

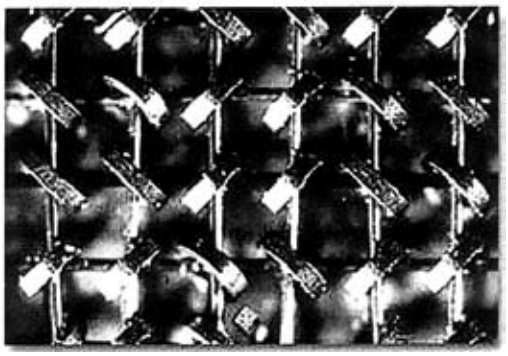
The authors would like to acknowledge kind assistance from Ewa Skrzypczak-Jankun, and Craig J. Eckhardt in preparing this and a special thanks to Mátyás Czugler for providing photos from the 1986 IUCr symposium in Beijing.

Tom J. Brett and
Jennifer M. Alexander-Brett

Forty years of struggle with computers over crystallography & intermolecular interactions

from the Kenneth N. Trueblood Award Lecture by Angelo Gavezzotti, University of Milano, Italy

Names are sounds, and metrics have been the lustre of poetry until about a century ago. When I entered Massimo Simonetta's Crystallography lab at the University of Milano in 1967 to start my thesis for the Italian *laurea* in chemistry, the magic sound in the air was a beautiful dactyl - spondee pair, the *clausola* of a Virgilian verse: Scho / màker and / Trùeblood. We had an IBM 1620 computer in good working condition, a microdensitometer that helped the visual reading of dark spots on films, and a new



Ferrite rings: the core memory of the IBM1620 (1967). Each ring is a bit.

automatic diffractometer, that was supposed to collect intensity data and to record them directly on punched cards. Rigid-body TLS analysis was no longer a voice coming from the promised land beyond the ocean, but could be carried out in our home for a small molecule, at the investment of only a few months' work. We were working in a bad-smelling basement because the upper floors could not carry the load of the hundreds of kilograms of mineral oil in which the transformers of the time had to swim, but the morale was as high as could be. We had to toil and sweat but we were the only ones around who could actually 'see' molecules.

For my thesis work, in those times one crystal structure determination, my supervisors were bold enough (with due respect, in hindsight: crazy enough) to tackle 1,1-di-*p*-tolylethylene, no heavy atom, no handle for the solution of the phase problem. My crystals were very thin, the diffractometer turned out to be dangerously prone to drifting into uncharted parts of *theta*/*chi* space, rather than falling onto Bragg spots; so the data had to be collected again from scratch and I eventually found myself with a bunch of Weissenberg photographic plates, no densitometer, because that was already in use for another project, and a few strips of film with graduated darkness scales to be matched to my diffraction spots. This took care of the next few months of my doctoral thesis work.

Massimo Simonetta, my scientific "father", had excellent connections with Caltech, having enjoyed there the fabulous season of the Pauling group in the 1950's - so in a way I can say that Ken and the former winner of his prize, Dick Marsh, are my scientific "uncles". Ken sent us a program written by a doctoral student in his group, Bob Long, that was supposed to solve the phase problem by a sort of necromancy called direct methods. We called it familiarly the "Trueblood" program. I studied the program instruction by instruction and wrote a detailed block diagram on the back of the diffractometer's roll of recording paper (probably the most useful part of the whole machine). We then ran the program in the shadows of mild scepticism, but later, when I made a "graphic" display of Fourier peaks using black paper balls sliding up and down a knitting needle to represent the atoms, much to the astonishment of the whole laboratory we saw that the structure had been solved. A degree, a preliminary communication in *Angewandte Chemie* and a full paper in *Acta Crystallographica* were granted.

Carol Brock and Ken on the background of the Iron Curtain (near Hamburg, 1984)

So the end of my thesis dealt only with the second part of the famous duo - I have never been so fortunate as to really meet the other half. But I did make progress with Ken. We got in touch by mail and exchanged software - which in those days meant sending around a large mag tape to convey a few hundred Fortran instructions. He and Emily Maverick were so kind as to place "a few remarks" on one of my manuscripts (which meant two pages, typewritten in small font). Ken and I finally met at the IUCr Congress in Hamburg, 1984. I learned to enjoy Ken's bright smiles. Then there were two occasions on the magic hill, in the bright sun of Erice, where I also had the fortune of getting to know lovely Jeanie.

Around the early 1980's Simonetta wanted to make a theoretical chemist out of me. Those were times in which a young man could hardly say no to a professor, and as a result I am a born crystallographer with a good acquaintance with quantum chemistry. The transition to an interest for intermolecular potentials was a natural one. Of course, in these times doing molecular orbital calculations still meant preparing by hand an input list with hundreds of Gaussian coefficients and exponents, and crystal calculations were out of the question, so we settled for the much handier atom-atom potential method. With Giuseppe Filippini we recalibrated our potentials so that observed average intermolecular radii would fit the position of the minima and experimental heats of sublimation would fit the potential energy wells. We were the first to have the patience to collect thousands of crystal structures and hundreds of thermochemistry data. We decided we would do without atomic point charges, and as a result I was burned at the stake at several meetings for such a heresy. But our potentials worked well and we were able to correct

a few mistakes in the literature of observed heats of sublimation by convincing Jim Chickos to re-determine some values that were at unexplained variance with our calculations. Giuseppe is also in a way my social *alter ego*. For example, one evening we were together at a banquet in a highbrow Cambridge college, and when I realized I had to sit at the high table and I was not wearing a tie he produced from his pocket an extra one he had brought for me, in what he knew was a very likely occurrence.

The author, a beaming Jack Dunitz and a busy Barbara Dunitz in 2003. Photo courtesy of Jay Siegel.

In the mid-eighties I was bold enough to apply the potentials to the prediction of crystal structures from scratch, nothing less. That obviously did not succeed, but by generating hundreds of crystal structures for any given molecule I was able to show that all observed crystal structures must be close-packed, but not all close-packed structures must be observed; this also meant that crystal polymorphism is a matter of lattice-energy differences of a few kJ/mol, something that many sensible crystallographers already suspected. We turned to the thermochemistry literature

The author and Giuseppe Filippini at the times of struggling with potentials.

on pharmaceuticals, where we found experimental proof that those differences can easily change sign upon change of authors, which we took to mean that they must not be too far from zero. In the late 1990's Jack Dunitz and Bernd Schweizer used my PROMET software for the Cambridge blind tests on crystal structure prediction. I sent them the source code with a detailed manual which they obviously did not read. Eventually, they supplemented the potentials with atomic point charges for which the method had not been calibrated. With patchwork potentials and a ridiculous software that fitted on a floppy disk they got two hits, one of which had the best accuracy of the whole lot of predictors. After such a coincidence I was more and more benignly looked upon from Zürich, an astral conjunction which I strongly suspect has been behind my ranking high in the list of people who might have deserved a Trueblood prize.

At the dawning of the new millennium I had the idea of looking at crystals using full molecular charge densities. I developed a numerical integration procedure for the calculation of Coulombic, polarization, dispersion and repulsion energies and I applied this "PIXEL" method to pairs of molecules in crystals. Once again, I was smart enough to convince Jack that the thing made sense, and we wrote together several papers debunking unjustified views on "structure-defining" interactions as we realized that the energies involved in these contacts were just tiny fractions of the total cohesive energies of the crystal. The PIXEL software is now adrift around the world and helping crystallographers to turn their structures inside out. One that I was not able to convince is Richard Bader, to whom I would like to pay my sincere respects for his elegant theory of Atoms in Molecules to which we all may have to surrender some day.

I have a prize, I have written a book that Oxford University Press has kindly published, so I'm ready for retirement in a couple of years' time, although the abstruse Italian regulations would allow me to hang around on full position and salary until the respectable age of 72. I think that the herd of mammoths blocking the road to young people is one of the worst evils of Italian Universities (there are many others), so I'll leave. Being a scientist has been a privilege perhaps undeservingly bestowed upon me and my gratitude goes to all the fellow scientists with whom I have shared this privilege. I love my wife Claudia for bearing with an aging computer addict like me. I convey my full sympathy to my old friend Gabor Somorjai for the Nobel prize he so deeply deserved and outrageously did not receive. I thank the ACA officials, the prize committee, as well as all the marvelous people at the meeting in Salt Lake City, Carol Brock and Joel Bernstein above all. Thanks are due to the people who spoke at the symposium, among them especially to Mike McBride for sharing with me over the years his untamed and far-reaching wit. I thank the ACA staff for being so kind and cooperative with the bureaucracy.

O reader, especially if you are under 30, think of people like Ken Trueblood who liberally served the ideal of pure science where curiosity and intellectual freedom reign unchecked, and remember: out there in the money-making world there is satisfaction, but often also weeping and gnashing of the teeth.

Angelo Gavezzotti

Editor's note: Angelo's book "Molecular Aggregation: Structure Analysis and Molecular Simulation of Crystals and Liquids" was described on page 22 of the spring 2007 ACA RefleXions.

Wanderings in the Fields of Chemical Crystallography

Frank H. Herbstein, Schulich Faculty of Chemistry, Technion–Israel Institute of Technology, Haifa, Israel

I have already expressed my appreciation of the ACA's 2007 Fankuchen Award and written a biographical sketch of Fan' (*ACA Reflexions*, Spring 2007,16–17). A much extended version of my talk in Salt Lake City is published in *Crystallography Reviews,* March, 2008, under the revised title "Classification of closed shell TCNQ salts into structural families and comparison of diffraction and spectroscopic methods of assigning charge states to TCNQ moieties," so I decided to give here some autobiographical background to 60-odd years of chemical crystallography.

I was born in Cape Town in the Union of South Africa (as it then was) on 3 July, 1926. My studies at the University of Cape Town (UCT) were interrupted by a year as a radar mechanic attached to the South African Air Force. After Hiroshima and Nagasaki I returned to UCT convinced that "physics was the future". R.W. James, FRS (*The Optical Principles of the Diffraction of X-rays*) was Head of Department and among my contemporaries were two future Nobel Prize winners - Sir Aaron Klug, P-PRS, and Alan Cormack. By the end of 1947 I had presented a master's thesis at UCT describing my unsuccessful attempts to solve the crystal structures of *o*-dinitrobenzene and a picric acid complex of an outlandish aromatic hydrocarbon whose name I have forgotten. But the die was cast -*o*-dinitrobenzene succumbed to my colleague Moshe Kapon in 1990 and I have (with others) solved the structures of many charge transfer (CT) compounds of aromatic hydrocarbons.

In the middle of 1948 I left Cape Town for the War of Independence in Israel, served in the Science Unit of the nascent Israel Defence Army and stayed on at the Weizmann Institute after the War as one of Gerhard Schmidt's first graduate students. Schmidt was an Oxford trained organic chemist with interests in biological crystallography, a student of Dorothy Hodgkin and now well known as a pioneer of 'crystal engineering,' a burgeoning career cut short by his premature death. I was too early to participate in Schmidt's photochemical studies -I worked on overcrowded aromatic hydrocarbons and the 3D structure of phenazine. After completing my Ph.D. in Rehovoth, I moved to MIT in the early 1950s; BE Warren was then the dominating influence in physical crystallography and I learned there that diffraction space extended far beyond the Bragg spots. This rather catholic education was later amplified by sabbaticals at Caltech and Northwestern in the United States, Cambridge and the Royal Institution in the UK and in South Africa at UCT and the University of the Witwatersrand.

After MIT I returned to South Africa in 1956 to join the staff of the South African Council for Scientific and Industrial Research (CSIR), an ambitious attempt to combine high quality academic and applied research. I enjoyed my nine years in Pretoria and published structures of some overcrowded halogenated aromatics and CT molecular compounds. The great goal of South African research in those days should have been directed towards understanding the mechanism of the Fischer-Tropsch process for converting low grade coal to petroleum products; we made some contributions but it was too large a project for our limited resources. I was fortunate enough to have left before the traumatic breakup of the CSIR, in the name of budgetary efficiency, got underway -how difficult to build, how easy to destroy.

A new chapter in my life started when, in 1965, I was invited to add an x-ray diffraction facility to the Department of Chemistry at Technion in Haifa; I became an Emeritus Professor at the end of September, 1994, but have continued in research. To my previous interests I added much more sophisticated approaches to topics that I had touched on earlier. Phase transitions was one of these. Second order transitions were the first to be developed; the simplest (a dangerous word) of these was the second order transition in naphthazarin C, studied in collaboration with Curtin and Paul in Urbana and Mogens Lehmann in Grenoble, which led on to a study of the *cis*-enol system benzoylacetone over a temperature range of 9°to 300°K with Finn Larsen's group in Århus. Just before leaving South Africa I had worked on a second order phase transition at ≈160°K in the CT compound pyrene: pyromellitic dianhydride and this work was greatly extended, including a structure determination at 19°K, during a sabbatical at Caltech with R. E. Marsh and Sten Samson. This led on to a review of second order transitions published in *Crystallography Reviews*, (2000),Vol. **5**, 181–226. The first order transitions in N-anilinophthalimide and N-(N'-methylanilino)phthalimide, first studied in the early years of the 20th Century, then attracted our attention; we were able to confirm the earlier results and relate them to thermodynamic properties of the system (*Acta Cryst.* (1998) **B54**, 277–290). A comprehensive view of enantiotropic first order transformations is given in the first part of Yuri Mnyuk's book *Fundamentals of Solid State Phase Transitions, Ferromagnetism and Ferroelectricity*, and we were able to put some of the phase transition material in a broader and more up-to-date context ("On the mechanism of first-order enantiotropic solid state transitions: from Simon through Ubbelohde to Mnyukh").

Two other consequences of my sabbaticals at Caltech must be mentioned. Following the pioneering studies of Dick Marsh and David Duchamp, Marsh and I (and others) were able to put much of the rather intricate crystal chemistry of trimesic acid on a sound basis. And Marsh taught me how to recognize potential space group errors and how to correct them with a smile. Jointly and severally this has led to re-assignment of correct space groups to more than 100 crystals and, indeed, to a recognition that there are errors in the literature not involving space groups and these too need attention.

I confess to developing an early penchant for writing Reviews; looking backwards and around helps to put looking ahead in perspective. Jack Dunitz encouraged me to write a review on "Crystalline Molecular Compounds: Chemistry, Spectroscopy and Crystallography" in the (lamentably defunct) *Perspectives in Structural Chemistry* and this, after many years, became part of a much broader two volume monograph entitled *Crystalline Molecular Complexes and Compounds (Structures and Principles)*.

What is my favorite piece of work? Undoubtedly "Spontaneous deformation of protocatechuic acid (3,4-dihydroxybenzoic acid) monohydrate (PCA.H_2O) crystals: crystallographic aspects" (Agmon & Herbstein, *Proc. Roy. Soc. Lond.* (1983), **A387**, 311–336), despite its being one of the least cited papers in the crystallographic literature. The unusual crystallization behaviour of PCA.H_2O was first reported in 1890 (and in 1905) by Otto Lehmann (a pioneer of liquid crystals), followed by a paper in the *Proceedings of the Royal Society of London* (1949) **A197**, 283–294 by Robert W. Wood a Professor of Experimental Physics at Johns Hopkins University, and author of *Physical Optics* (first published in 1911). This was Wood's last publication, at age 81, and my guess is that it was in response to his election as a Foreign Member of the Royal Society. Neither Lehmann nor Wood realized that they were dealing with the monohydrate. Ilana Agmon and I were able to confirm their observations and put them into a rational crystallographic framework. And what are my favorite crystals? Here trimesic acid and the various polyidides (and polyiodines) run neck and neck.

An important lesson from this rather dispersed list of topics, appreciated by more and more crystallographers, is that much is to be learned from studies over a wide range of temperatures (and pressures) -one needs to cover as much as possible of P–T phase space instead of restricting one's efforts to 298°K, 1 bar.

Acknowledgements: There are others, not mentioned explicitly above, who have contributed significantly. Jan Boeyens and Ferdi de Wet, (both then at CSIR), (the late) David Ginsburg, who invited me to Haifa and with whom I collaborated on propellane crystallography, and my Haifa colleagues in the x-ray laboratory Ilan Goldberg, Moshe Kapon, Mark Botoshansky, George Reisner and Menahem Kaftory

Frank Herbstein

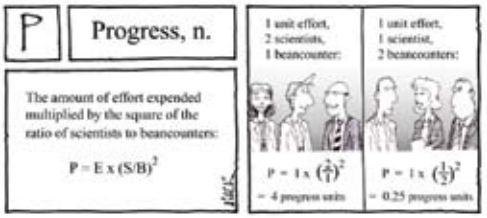
Nanoscience images from ORNL. From left: Ga ball-Si crystal-SiOx nanowire octapus; ZnO combs; ZnO nanowire fireworks; ZnS embroidery.

Contributors to This Issue

Cele Abad-Zapetero, Jennifer Alexander-Brett, Tim Barnett, Ernst Bergmann, Gloria Borgstahl, Katie Bowman, Tom Brett, Jim Britten, Branton Campbell, Jamie Cate, Bryan Chakoumakos, Marcia Colquhoun, Mark Collins, Bryan Craven, Angelo Gavezzotti, Richard Gillilan, Angie Grossen, Marvin Hackert, David Harrison, Frank Herbstein, Jason Hodges, John Horton, Andy Howard, Bobby Huether, Ashfia Huq, Lisa Keefe, Amy Kendall, Herbert Kiel, Charles Lake, Cora Lind, Bruce Noll, Doug Ohlenberg, Joseph Orgel, Thomas Proffen, Claudia Rawn, Alec Sandy, Steven Sheriff, Gerald Stubbs, Dale Swenson, Jack Tanner, Bi-Cheng Wang, Pamela Whitfield, Carrie Wilmot.

Index of Advertisers

Progress
by Nick D. Kim, U. Waikato, New Zealand. See nearingzero.net/res.html.



winnner of the New Product Award at
LabAutomation2008

Formulator™

Next-generation liquid handler

Dispense 96-well grids in 60 seconds

The Formulator™ is a next-generation liquid handler that uses microfluidics to dispense screens and optimizations up to **ten times faster** than any other liquid handler available today.

FORMULATRIX
Makers of
Rock Imager Rock Maker

Info: +1 781-788-0228, Fax: +1 781-207-5522, info@formulatrix.com www.formulatrix.com

Picasso encounters crystallography: An unique excursion into the intersection between the Sciences and the Arts.

From left: Cele Abad-Zapatero as Pablo Picasso, Karl Volz as J.D. Bernal, Andrew Mesecar as W.L. Bragg, George Chlipala as J.B.J. Fourier, and Aimée Eggler as Rosalind Franklin. Photos are from the first reading of the play, courtesy of Aimée Eggler, Yahira Baéz and Kelly Gay.

In our daily routine as committed scientists devoted to our professions, we tend to forget how much our imagination, dedication and drive resemble the efforts of artists in their daily struggle. In addition, we tend to forget that while our specialized toil affects people's lives, they do not understand what we do. To address these key issues, the APS is planning to present a unique event to inaugurate its 2008 Annual Users Meeting May 4th-8th. The framework is provided by a new play entitled *Picasso Meets Crystallography* recently read at University of Illinois at Chicago (UIC) that centers on the historical meeting between Picasso and J.D. Bernal in 1950.

Coincidentally, on January 14, 2008 the mural ('Sage') drawn by Pablo Picasso in London in 1950 at the flat of J. D. Bernal, the most charismatic crystallographer of his generation, was unveiled at the headquarters of the Wellcome Trust in London. This unique artistic record of the meeting of these two giants was left behind by Picasso at Bernal's flat at Birbeck College on November, 12, 1950. The mural was dismantled when the building at 21 Torrington Square was demolished and was housed temporarily at the Institute of Contemporary Art in London, until the renovations of Birbeck were completed in 1998.

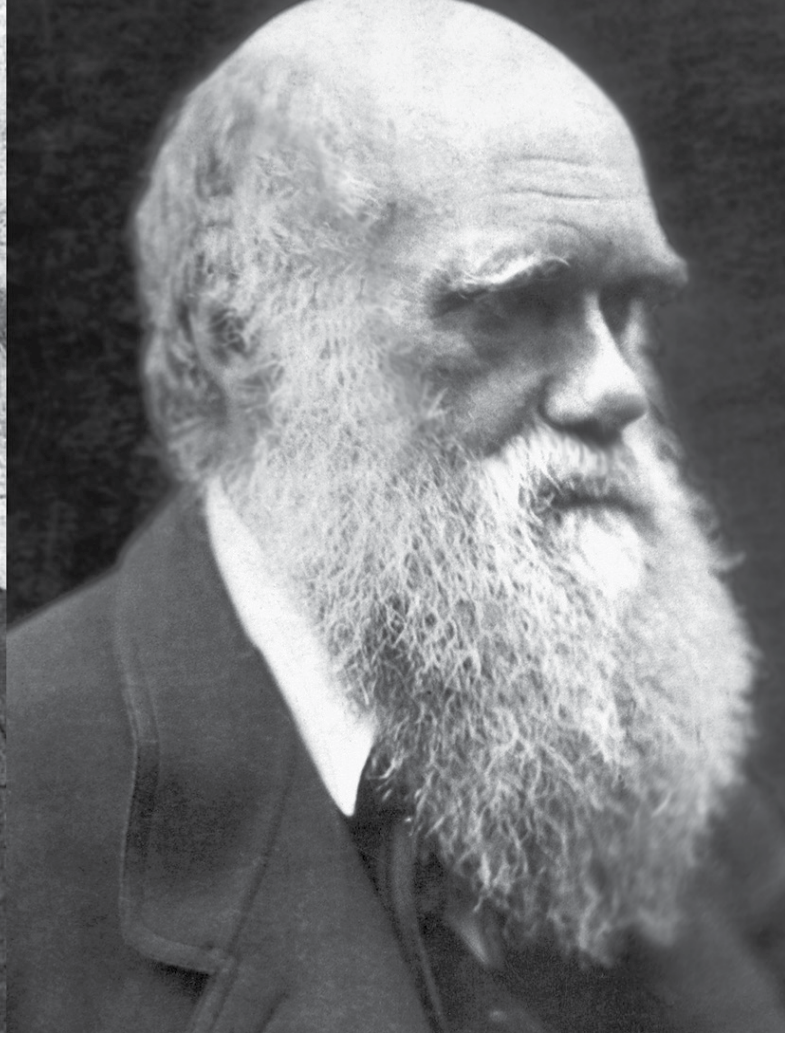
Picasso and J. D. Bernal together? What brought these two iconic figures of the Arts and the Sciences together? What did they talk about? Crystallography and Art? Politics? The tribulations and romantic problems in their lives? Answers to these questions and others form the texture of the play *Picasso Meets Crystallography*. Through this dramatic structure the play attempts to provide a forum for the dialog and discussion of the connections and differences between the sciences and the arts, the origins of molecular biology and related themes. Besides Picasso and Bernal, the characters of the play are Rosalind Franklin, J.B.J. Fourier and W.L. Bragg.

This play is certainly not the first one dealing with scientific heroes or science-related themes. I would like to bring to the attention of younger crystallographers (or scientists at large) just a few landmarks of the genera of plays having to do directly or indirectly with science. In my student days in Spain, I was mesmerized by *Life of Galileo* (1939, 1947), the masterpiece of the German playwright Bertolt Brecht centered on the life and conflicts of Galileo. The social responsibility of scientists in society resulting from the development of atomic energy was explored by the Swiss playwright Fiedrich Dürrenmatt in *The Physicists* (1962). More recently the intriguing brief play entitled *Oxygen* (2000) by Carl Djerassi and Roald Hoffmann addresses the issue of who really discovered oxygen, Lavoisier, Sheele or Priestley. Finally, I would draw attention to the subtle and enormously successful play *Copenhagen* (1998, 2000) by Michael Frayn, which attempts to recreate what really happened in the historical meeting between Niels Bohr and Werner Heissember during WW II. A recent book entitled *Science on Stage* by Kirsten Shepherd-Barr, Senior Lecturer at the University of Birmingham, UK (Princeton University Press, 2006), discusses the trends in this unique area of science-writing and reviews and comments on more than one hundred plays presenting scientific themes on stage.

Although the script is still being developed, the first complete reading of *Picasso Meets Crystallography* took place on December, 14, 2007 at the Center for Pharmaceutical Biotechnology of the UIC. The cast of characters was as follows: J. D. Bernal: **Karl Volz**; W. L. Bragg: **Andrew Mesecar**; J.B. J. Fourier: **George Chlipala**; R. Franklin: **Aimée Eggler**; Pablo R. Picasso: Cele Abad-Zapatero. Cele was author and director, and stage directions were by **Valerie Grum-Tokars**. Supporting staff were: **Yahira Baéz** and **Kelly Gay** for images and video; **Jacqueline LaMarre** for music and audio; **Yang Tian** (with the assistance of Valerie Grum-Tokars) for stage setup; **E. Woods** and **Y. Yong** for signs and leaflets. Additional photos of the reading are at **http://picasaweb.google.com/aimee.eggler/TheReading**).

We invite the crystallographic community to bring this historical meeting alive by supporting the full stage production at the premiere of this play which will take place during the opening of the APS 2008 Annual User's Week Meeting on May 4. In addition, a documentary will be filmed that will illustrate the relation between the sciences and the arts and help to communicate to the lay public what we do as scientists and as human beings. Individual, organizational and corporate contributions are invited and will be welcomed. The project is supported in part by the IUCr. Further information about this unique project can be found at: **http://www.aps.anl.gov/Users/Meeting/2008/Picasso/index.php** or by e-mail to **caz@uic.edu, or strasser@aps.anl.gov.**

Cele Abad-Zapatero



Are Wyatt instruments the product of intelligent design or evolution? Yes.

There's no debate about it. We *invented* commercial laser light scattering, then built on it to develop a complete family of related instruments, all of which provide unparalleled performance for our customers.

Today, Wyatt's light scattering products are *the* most widely recognized on earth. Thousands of chemical, biotechnology, pharmaceutical, academic and government laboratories around the world rely on them to characterize macromolecules of all kinds. Just some of these examples have been published in *over* 2,500 peer-reviewed articles based on their work using Wyatt instruments. These articles, application notes and other feedback in the scientific environment have helped our 15 PhD scientists and other innovators to refine our instruments more rapidly to meet our customers' needs. And oftentimes, the result is an unprecedented new product.

So, was it intelligent design or evolution? Precisely.

For more information call 805.681.9009 or visit us at **www.wyatt.com**.

Wyatt Technology CORPORATION

DAWN HELEOS. The most advanced commercial light scattering instrument for macromolecular characterization.

Optilab rEX. The refractometer with the greatest combination of sensitivity and range.

ViscoStar. The viscometer with unparalleled signal-to-noise ratios, stable baselines and a 21st-century interface.

Eclipse. The ultimate system for the separation of proteins and nanoparticles in solution.

DynaPro. The world's most popular dynamic light scattering instrument for protein and nanoparticle characterization.

Update on Climate Change

Jan. 31st, 2008: A team led by **Tim Barnett**, a climate expert at Scripps, published a definitive study in *Science Express*: ***Human-induced Changes in the Hydrology of the Western United States***, Tim P. Barnett, *et al*, that concludes (with likelihood between 0.01 and 0.001) that up to 60% of changes in three key factors affecting the West's water cycle, river flow, winter air temperatures and snow pack, are due to human-caused climate change. In their careful study, they used a high-resolution hydrologic model forced by global climate models. Their results "portend, in conjunction with previous work, a coming crisis in water supply for the western United States." Furthermore, a more recent study (T.P. Barnett, D.W. Pierce, submitted for publication in *Water Resources, Research*), "puts the timing of this impact within the next 10-20 years with high probability."

From ***Trouble in Them Thar Hills***, by Phil Berardelli, *ScienceNOW Daily News*, 12th Dec, 2007: Glacier National Park in Montana, which once boasted 150 spectacular rivers of ice, is now down to 25. Daniel Fagre, an ecologist at USGS's Northern Rocky Mountain Science Center, reported at a meeting of the American Geophysical Union that recent data show that the remainder "may be gone in our lifetimes." One of the hardest hit is the Grinnell Glacier, which had ice as much as 300 meters thick when it was discovered in the 19th century. Now that ice is completely gone in some places, exposing soils that have not seen daylight in thousands of years. Thomas Painter, U.Utah, reported that in addition to warmer temperatures, carbon black (soot) which continually rains down on the glaciers but tends to concentrate on the surface of the ice, increases heat absorption from the sun's rays by 43%.

Views of the Grinnell Glacier; top: 1900 (F.E. Matthes, Glacier National Park Archives); below: 1998 (Lisa McKeon, USGS.)

On a more optimistic note, *JACS* announced their March 19th, 2008 issue would include an article reporting the development of a new, low-cost material for capturing CO_2 from the smokestacks of coal-fired electric power plants and other industrial sources. ***Designing Adsorbents for CO_2 Capture from Flue Gas-Hyperbranched Aminosilicas (HAS) Capable of Capturing CO_2 Reversibly***, Jason C. Hicks *et al*, was published on the web, *JACS Communications*, Feb. 19th. In this study, Christopher Jones, Georgia Inst. Tech., and colleagues describe the development of a new solid adsorbent combined with an HAS that would avoid the problems with existing technology. The new material captured up to 7 times more CO_2 than conventional solid materials, shows greater stability under different temperature extremes, and can be recycled numerous times.

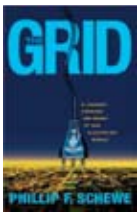
Evolving Methods for Macromolecular Crystallography: The Structural Path to the Understanding of the Mechanism of Action of CBRN Agents **NATO Science Series II: Mathematics, Physics and Chemistry**, Randy J. Read and Joel L. Sussman, Eds. Springer; hardcover: June, 2007, 191 pp. $116.07; IBSN: 1402063148; paperback: March, 2008, 191 pp. $69.95, IBSN: 1402063156.

This volume draws on the expertise of leaders in the field of macromolecular crystallography to describe developments that are accelerating progress in structural biology. Contributions span the range of techniques from crystallization through data collection, structure solution and analysis, and show how modern high-throughput methods are contributing to a deeper understanding of medical problems. The final chapter is a review by **David Sayre**, (who will receive the 2008 Ewald Award at the IUCr Congress in Osaka) on the current status of single-particle x-ray imaging. The 2D images of a quick-frozen yeast cell obtained in the Stony Brook/Cornell/Berkeley single yeast cell imaging project are described. If 3D images could be obtained at the same resolution, they would allow observation of the positions of the large molecular assemblies in an entire almost-living-state cell.

The Weather Makers : How Man Is Changing the Climate and What It Means for Life on Earth by **Tim Flannery**. Hardcover: Atlantic Monthly Press (2006), 384 pp., $16.32; IBSN: 0871139359; paperback: Grove/Atlantic, Inc. (2007), 359 pp. $13.50. IBSN: 0802142923.

Tim Flannery, a paleontologist and global warming activist, is an adjunct professor at Macquarie University in Australia. According to a Kliatt review, *The Weather Makers* was written in 2004 but he wrote afterwards in 2005 and 2006 updating his dire predictions and indicating that global warming is happening even faster than predicted. "...he projects three possible ways global warming will ultimately occur: through the collapse of the Gulf Stream, the collapse of the Amazon rain forests, or methane release from the ocean floor and points out that humans can only control these events if they do something now, without waiting for further proof." The book is thought by several reviewers to be somewhat less objective than Elizabeth Kolbert's *Field Notes from a Catastrophe: Man, Nature, and Climate Change*, (2006) which was described in the Books section of the spring 2007 *ACA Reflexions*.

The Grid: A Journey Through the Heart of Our Electrified World, by Joseph Henry Press (2007) hardcover, 320 pp. $18.45; IBSN: 030910260X.



Phillip Schewe, a particle physicist, is the chief science writer at the AIP. He also is a playwright (and a member of the Dramatists Guild). *The Grid* is an historical account of the electrical grid, from Thomas Edison's time to the present, and tells many interesting stories -tales about the 1965 blackout, and about an Idaho Power transformer-repair field trip are two examples. A review in *Physics Today* (Feb. 2008, p. 63) is generally favorable, but faults the book for somewhat "peculiar" organization and for it's dramatic and philosophical bent (numerous quotes from Lewis Mumford and Henry David Thoreau). However, the electrical grid is a fascinating construction, and one that is mysterious to many of us, so this book is welcome.

ACA 2008 May 31st – June 5th,
Knoxville Convention Center, Knoxville, TN



PROGRAM CHAIRS

Paul Butler
NIST, Gaithersburg, MD
301-975-2028
aca08@ornl.gov
Fax 301-921-9847

Dean Myles
ORNL, Oak Ridge, TN
865-574-5662
aca08@ornl.gov
Fax 865-574-8363

LOCAL CHAIR:

Jason Hodges
ORNL, Oak Ridge, TN
865-576-7034
aca08@ornl.gov
Fax: 865-574-6080

Advance Registration Deadline: April 4, 2008

Advance Hotel Registration Deadline: April 15, 2008

Register online and see Abstracts online at **www.AmerCrystalAssn.org** ***Questions:*** **aca@hwi.buffalo.edu**

Registration fees

Fee	Advance (before April 4)	Late (after April 4)
Regular Member	$395	$595
Retired Member	$161	$239
Post doc Member	$200	$298
Student Member	$161	$235
Nonmember*	$590	$883
Post doc Nonmember*	$298	$444
Student Nonmember*	$239	$356
Guest**	$ 50	$ 50
WK.01	$120 (for all)	
WK.02	$100 ($60 students)	
WK.03	$110 ($60 students)	
WK.04	$110 ($70 students)	
Mentor/Mentee Dinner		
Mentor	$30	
Mentee	$20	
Banquet	$55 ($25 students)	

* The nonmember registration fee includes a complimentary membership to the Association for 2008. Those registering as nonmember post docs or nonmember students must include documentation of this status with registration form.

**Guest registration includes the opening reception, exhibit show and get together on Sunday morning.

2008 ACA Meeting Climate Neutral Campaign

We hope that members and sponsors of the ACA will join our effort to make the 2008 meeting Climate Neutral. We cannot prevent all greenhouse gas emissions, but we can ensure that the net result of our activities decreases rather than increases the amount of CO_2 in the atmosphere. This goal can be achieved by offsetting the CO_2 released as a consequence of attendees and vendors flying to the meeting and use of the conference center and hotels. We plan to do this by continuing the campaign begun last meeting. We have selected the national Carbonfund organization to make the ACA 2008 annual meeting a CarbonFree event. **Carbonfund.org** is dedicated to fighting climate change, making it easy and affordable for any person or organization to eliminate their climate impact and hastening the transformation to a clean energy and technology future. They work to achieve this by providing climate change education and cost-effective solutions to carbon reductions that include saving energy and carbon offsets.

The **ACA 2008 Climate Neutral Campaign** will use the carbon offsets program of **Carbonfund.org** to help compensate the CO_2 emissions associated with this meeting. Our purchases of carbon offsets will support three types of carbon offset projects: renewable energy, energy efficiency, and reforestation. While each is different, they all play an important role in the fight against climate change. All offset obligations are matched against projects that meet or will meet the Climate, Community and Biodiversity Alliance, Environmental Resources Trust, or United Nations Framework Convention on Climate Change Joint Implementation (JI) standards. Detailed information on the different types of carbon offset can be found at the **Carbonfund.org** website.

Carbonfund.org

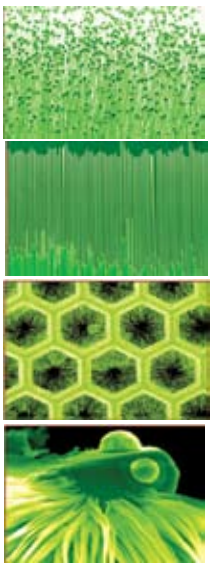
Preliminary estimates indicate that to make our ACA 2008 meeting Climate Neutral we will need to offset 475 tons of emissions or approximately 1600 lbs for every attendee (84% of the emissions are travel, the remainder hotel, venue and meals). An average purchase of $4 of carbon offsets per attendee will allow us to reach our goal. After completing the ACA 2008 meeting registration, contributions can be made on the ACA web page which is setup to collect and track the effectiveness of this campaign.

Jason, Paul and Dean

Special Event - Tour of the Spallation Neutron Source

On Sunday evening, June 1st, there will be an Oak Ridge National Laboratory sponsored tour of the Spallation Neutron Source including hors d'oeuvres and refreshments. Pre-registration is required.

The Spallation Neutron Source (SNS) is the first of a new generation of spallation neutron user facilities, exemplifying a significant increase in both neutron production power and instrument technology. Currently ramping up to full power, the SNS is already producing the world's most intense pulsed neutron beams for materials, physics, chemistry and biological research. The SNS is currently building and commissioning a diverse suite of eighteen instruments for diffraction, small-angle scattering, spectroscopy and reflectometry. These complement the scattering instruments at the recently upgraded High Flux Isotope Reactor (HFIR) neutron source. For more information on both the SNS and HFIR neutron user facilities, please visit **http://neutrons.ornl.gov.**



Nanoscience images from ORNL. From the top: Germanium-catalyzed ZnO nanowire forest; ZnO combs; Germanium-catalyzed ZnO nanowire on copper grid; Ga balls-Si crystal-SiO_x nanowire sandwich .

Registration for the tour is open to ACA 2008 attendees and exhibitors only; there is no charge for this event. Charter buses will bring attendees to the SNS and back. An ACA 2008 conference badge will be needed to board the buses. All participants in this special tour must register prior to 1st May 2008. Tour registration can be completed online by following the SNS tour link on the left side of the ACA 2008 website at **neutrons.ornl.gov/conf/aca2008**.

Workshops, Saturday, May 31st

WK.01 Magnetic Structure Analysis by Neutron Diffraction Techniques
WK.02 Neutron Macromolecular Crystallography from Expression to Refinement
WK.03 Wise Use of Dose: Structure Solvability vs Structure Integrity
WK.04 Structural Biology Without Crystals: Small Angle Scattering Methods

Award Symposia

Pattterson Award in honor of Bi-Cheng Wang, *organized by John Rose and Gary Newton and sponsored by the BioMac SIG*

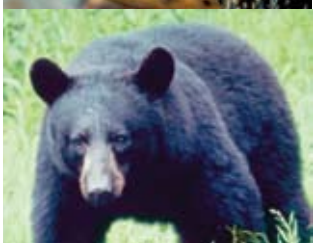
Margaret C. Etter Early Career Award to honor Radu Custelcean, ***organized by Anna Gardberg and sponsored by the General Interest and Young Scientist SIGs***

Transactions Symposium

on Complementary Methods,

organized by Carrie Wilmot and Susan Kruger and sponsored by the BioMac, General Interest, Neutron Scattering, Powder Diffraction, SAS, and Synchrotron SIGs

Speakers: James Stivers, Kylie Walters, Oliver Einsle, James Holton, Jill Trewhella, Doug Tobias, Dominique Bourgeois, Leighton Coates, David Worcester, Shuji Akiyama, Joseph Wedekind, Carole Bewley



Great Smoky Mountains photos of the Eastern Box Turtle and Black Bear from nps.gov/grsm/photosmultimedia/index.htm

Exhibit Show 2008 An exhibition of the latest instruments and techniques for sample isolation, purification and preparation, crystal growth and data collection, computer software for data storage, retrieval analysis, graphics systems, databases, and books, journals and other materials essential to modern crystallographery is scheduled to begin on the evening of Saturday, May 31 in conjunction with the opening reception. The 2008 Show will run through Tuesday evening June 3. The exhibit show will be closed on Wednesday June 4th but posters will remain accessible. The Advertising and Exhibits Div. of the American Inst. of Physics is managing the show. For further information contact **Bob Finnegan,** AIP, 2 Huntington Quadrangle, Suite 1NO1, Melville, NY 11747, **rfinneg@aip.org,** ph. (516) 576-2433; fax (516) 576-2481. ACA Corporate Members will receive 10% off one booth fee. Not a member? Join now!Not-for-profits groups are eligible for a discounted booth fee of $400 for one booth. Booth rental is $1,400 for all others.

Register online at www.AmerCrystalAssn.org

MAY 2008

29-June 8 **From Molecules to Medicine, Integrating Crystallography in Drug Discovery** Erice, Italy.**www.crystalerice.org/erice2008/2008.htm.**

31-June 5 **ACA Annual Meeting -Knoxville, TN** ***Local Chair: Jason Hodges, ORNL, Program Chairs: Paul Butler, NIST, and Dean Myles, ORNL,*** **aca08@ornl.gov.**

30-June 13 **15th Pan-American Synchrotron Radiation Instrumentation Conference,** Saskatoon, Alberta, CA. ***www.lightsource.ca/medsi-sri2008***

JUNE 2008

3-6 **16st Annual Meeting of the German Cristallographic Assoc.**, Erlangen, Germany; **http://conventus.de/dgk2008/**; Contact: Herr Prof. Dr. Andreas Magerl, Friedrich-Alexander Universität Erlangen-Nürnberg, +49 (0) 9131 85 25 181; **andreas.magerl@krist.uni-erlangen.de.**

6-11 **5th European Charge Density Meeting (ECDM5)** - Palazzo Gallio, Gravedona, Italy, **http://ecdm5.istm.cnr.it/index.html**

18-22 **International Summer School - Structure Determination from Powder Diffraction Data**. Paul Scherrer Institut, Villigen, Switzerland. **http://user.web.psi.ch/powder08**

19-20 **Protein Crystallography Europe** Amsterdam, Netherlands. **www.selectbiosciences.com/conferences/PCE2008**

AUGUST 2008

21-28 **IUCr2008:** 21st Congress of the International Union of Crystallography, Osaka, Japan. **congre.co.jp/iucr2008.**

SEPTEMBER 2008

20-24 **ICSG 2008 International Conference on Structural Genomics**, Oxford, UK, ***www.spine2.eu/ISGO*** sponsored by ISGO, the International Structural Genomics Org. ***www.isgo.org***

JULY 2008

13-18 **Gordon Research Conference: Diffraction Methods in Structural Biology**, Lewiston ME USA. Bates College, Lewiston, ME. **www.grc.org/programs.aspx?year=2008&program=diffrac**

SEPTEMBER 2008

7-12 **BCA/CCP4 Summer School in Macromolecular Crystallography,** Oxford, UK. **www.biop.ox.ac.uk/www/bcasummer2008.html**

19-22 **EPDIC-11 European Powder Diffraction Conference** Warsaw Poland.**www.epdic-11.eu/**

JUNE 2009

4-14 **High Pressure Crystallography: From Novel Experimental Approaches to Applications to Cutting Edge:** Erice, Italy. **www.crystalerice.org/2009.htm.**

JULY 2009

25-30 **ACA Annual Meeting - Toronto - Ontario - Canada** ***Program Chair: Jim Britten (McMaster U.,*** **britten@mcmaster.ca*).***

AUGUST 2009

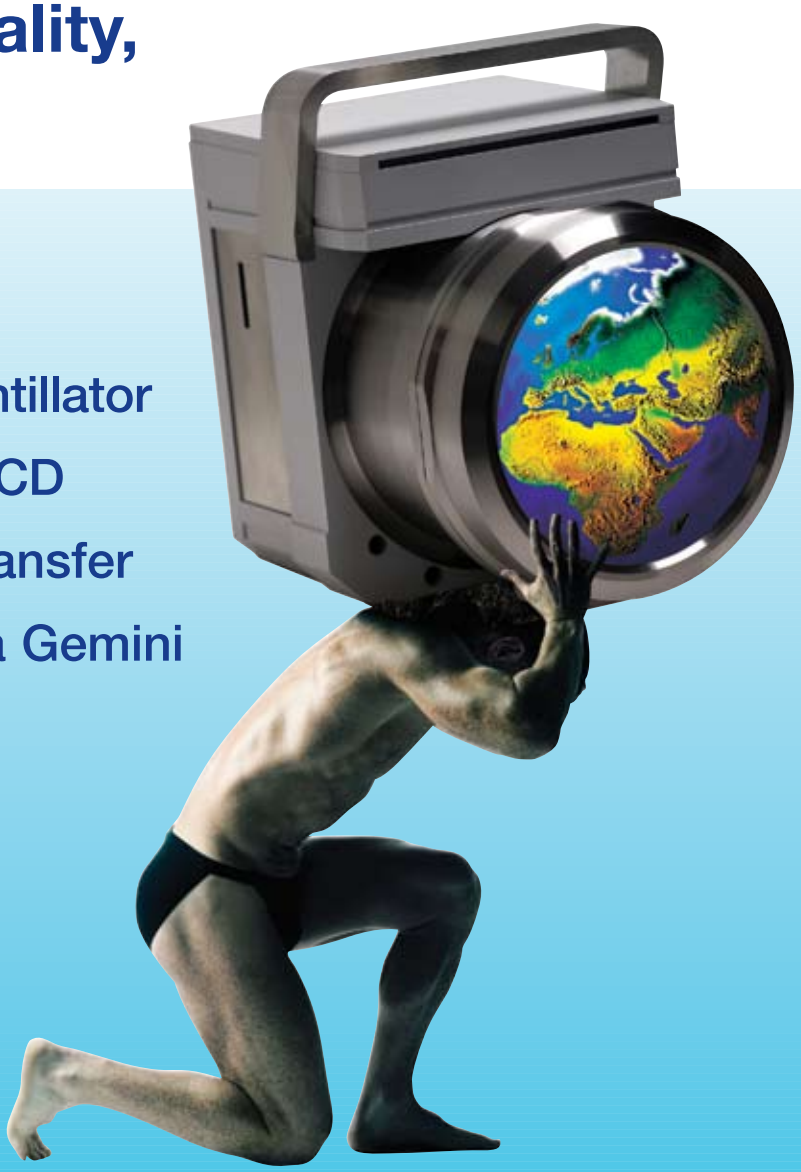
9-14 ***ECM-25 Istanbul, Turkey.***

oxford diffraction

driving X-ray innovation

NEW *Atlas CCD*

Ultimate data quality, up to 3.5x faster!



- 135 mm diameter, active area
- New ‘Super plus’ scintillator
- 4-port fast readout CCD
- 1Gb ethernet data transfer
- Available as part of a Gemini or Xcalibur system

sales@oxford-diffraction.com www.oxford-diffraction.com

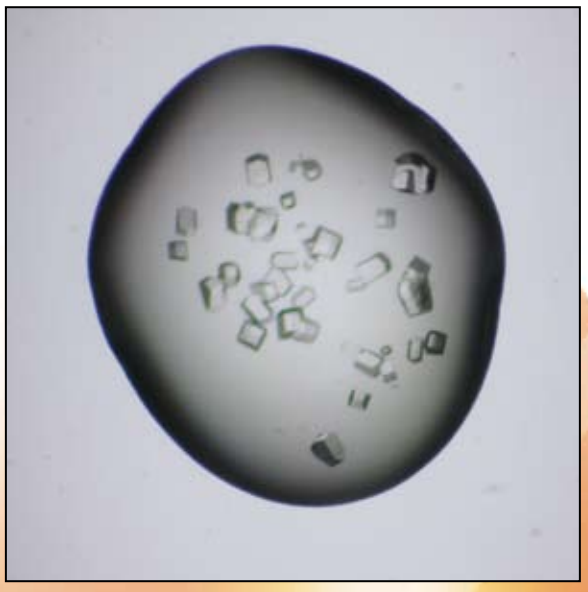
Europe Tel: +44 (0)1235 443630 Fax: +44 (0)1235 443631
North America Tel: +1 540 443 9272 Fax: +1 540 443 3672
Asia Tel: +852 2571 9188 Fax: +852 2571 9855

THE QUEEN'S AWARDS FOR ENTERPRISE: INTERNATIONAL TRADE 2006

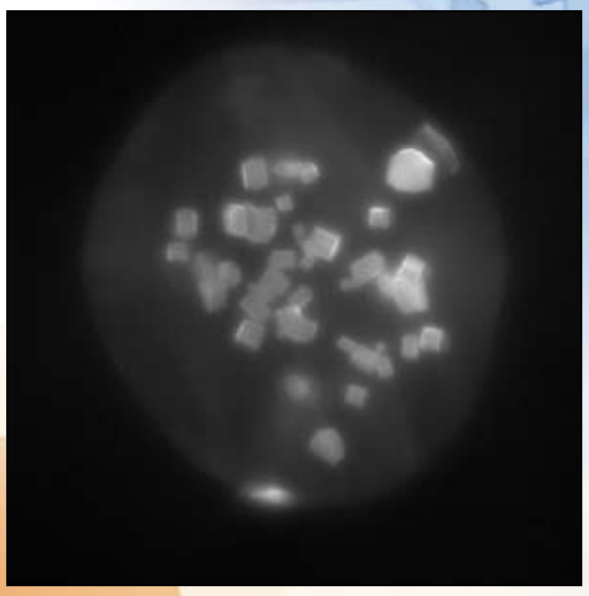
See what U'V been missing!

Leading With Innovation

Desktop Minstrel™ UV crystal imaging for protein crystallography



Visible light image



Ultraviolet light image

Screen your crystals quickly, accurately and automatically

www.Rigaku.com/automation

Rigaku

Rigaku Americas Corporation phone: 281-362-2300 e-mail: info@Rigaku.com
Rigaku Europe phone: +[44] 1732 763367