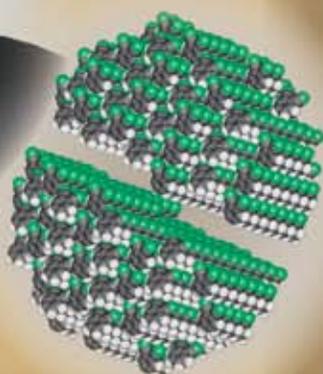


American Crystallographic
Association

ACA RefleXions

Number 1
Spring, 2007



2007 Awards
Kenneth Trueblood
Isidor Fankuchen

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ACA Reflexions

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Cover: see page 17
At the 2007 ACA Meeting, Angelo Gavezotti will receive the Kenneth N. Trueblood Award, and Frank Herbstein will receive the Isidor Fankuchen Memorial Award.



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

Connie Chidester..... Judith L. Flippen-Anderson
2115 Glenwood Dr 3521 Launcelot Way
Kalamazoo, MI 49008 Annandale, VA 22003
tel. 269-342-1600 tel. 703-346-2441
fax 716-898-8695..... fax 716-898-8695
conniechidester@earthlink.net..... 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
phone: 716-898-8692; fax: 716-898-8695
email: marcia@hwi.buffalo.edu

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President's Column:

The year 2007 is already proving to be an exciting one for the ACA, and I am looking forward to being involved in the activities described below. I will address the changes on council and the program for the upcoming meeting in Salt Lake City as well as future meetings and the international nature of our association. I will also make some predictions about the future health of our profession.

First I would like to express my gratitude, and that of the ACA, for the excellent service provided by Louis Delbaere and Doug Ohlendorf who are leaving their posts of Past-President and Treasurer respectively. Doug will be replaced by Bernie Santarsiero who I welcome to council and look forward to working with. My thanks also to my predecessor, Bob Bau, who has provided me with a solid apprenticeship, and whose experience will be a valuable resource over the next year. I also welcome our new Vice President, Marv Hackert, who is already actively participating in the affairs of council. It is also a pleasure to be working closely again with our Buffalo team who really are responsible for connecting all the dots so that the operation of the ACA appears seamless to the membership.

The culmination each year of the work of council and the Buffalo office is the annual meeting. This year we will meet in Salt Lake City in July (see pp. 30-31). The scientific program is rapidly coming together thanks to Jill Trehwella and the SIGs. A striking part of the program is the number of sessions that are interdisciplinary in nature and jointly sponsored. The meeting will again have a very international flavor, the Program Chair being primarily located in Australia, and several of the session organizers being based in Europe. Ah, the power of the internet! At this meeting, we will make a number of awards. The Fankuchen Award will be presented to Frank Herbstein (Haifa) and the Trueblood Award to Angelo Gavezzotti (Milan), and the symposia organized in their honor will have speakers from around the world. The Wood Award will go to Lisa Randall (Harvard) and the Etter Early Career Award will be presented to Cora Lind (Toledo). On the final day of the meeting, there will be a lecture from "our" latest Nobel laureate, Roger D. Kornberg; my thanks to local chair, Chris Hill, for successfully extending the invitation, and to Sue Byram (Bruker AXS) for underwriting this event.

Our next meeting will be a spring meeting in Knoxville, TN in 2008 (the Local Chair is Jason Hodges, and Program Co-Chairs are Paul Butler and Dean Myles). No doubt, the neutron scattering community will have the possibility of getting an up-to-the-minute status report on the new facilities currently under construction at Oak Ridge. This will be followed by a summer meeting in Toronto in 2009 (Jim Britten is Program Chair). The next Patterson Award will be made at the Knoxville meeting. Please see page 5 or our web site for the call for nominations.



I know that many of you are concerned about the future health of our crystallographic community. Thanks to a solid group of volunteers, the ACA is able to sponsor two summer schools – one oriented towards small molecules and the other towards macromolecules. The financial support from ACA for these schools has only been a year-to-year commitment in the past. In order to ensure continuity, council will be putting in place a mechanism to provide a longer term commitment in the future. How can you help to recruit the next generation of crystallographers? Bring your students and post-docs to our meetings to share in the excitement, and expose them to all of the areas of science where crystallography is making an impact. Low registration fees which include a student membership in the ACA, cheap and sharable alternative hotel accommodations, and student travel awards are all available to facilitate their participation.

I look forward to seeing you all by the Great Salt Lake at the foot of the Wasatch Mountains in July.

Alan Pinkerton

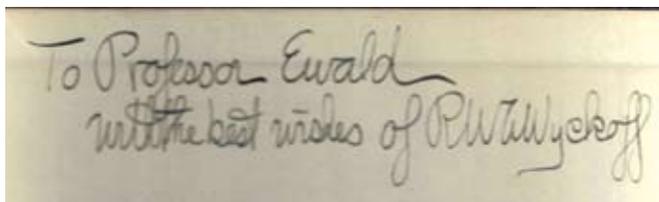
Letters to the Editor

Thank you very much for the nice news piece in the last issue of *ACA Reflexions* about the Etter Award! While I enjoyed reading it, I would like to point out that the article gives me too much credit: somehow, the word "powder" got lost in one of the sentences. I am the resident powder crystallographer at the University of Toledo, and I manage the powder x-ray facilities together with Pannee Burckel. Without this word, the article gives me credit for the excellent work of several of my colleagues: the Instrumentation Center has two staff crystallographers, Kristin Kirschbaum who oversees the small molecule diffractometers and is the director of the Center, and Leif Hanson, our staff macromolecular crystallographer, who

is in charge of the high brilliance diffractometer. In addition, in the Chemistry Department ACA President Alan Pinkerton and his group and macromolecular crystallographers Timothy Mueser and Donald Ronning all contribute to our list of "resident crystallographers."

Cora Lind

Editor's note: The article that Cora refers to was the announcement, in the winter *ACA Reflexions*, that she is to receive the 2007 Margaret C. Etter Early Career Award at our annual meeting in Salt Lake City.



Editor's note: With Scott's permission we are reprinting his letter to Alan Pinkerton in the hope that among our readers someone will recognize the handwriting and perhaps be able to shed some light on his mystery.

I'm writing to you with somewhat of an odd request and am hoping that since you are the ACA president, you might be able to point me in the right direction. I was recently sorting through some old books when I came across Wyckoff's *The Structure of Crystals* which I obtained some time ago. Please allow me to share this story with you. In 1996 I was still a graduate student in Bart Kahr's lab at Purdue University where I studied

the orientation of guest molecules in organic host crystals. My parents lived in Minneapolis at the time and when I visited them, I would often go to an antique bookstore in Stillwater, MN. Most of the time I would find some very interesting books. Especially scientific ones. One time in particular, I noticed Wyckoff's *The Structure of Crystals 2nd Edition*, 1931 which I had thumbed through on many occasions and thought it would be a good addition to my collection. When I opened the cover I noticed some writing which read "To Professor Ewald with the best wishes of RWG Wyckoff" (see figure). I hadn't really thought about it much until recently and was wondering if you might know of any sources that would have examples Wyckoff's handwriting. I'm interested to know if this is real or not. If it is authentic, one might wonder how it ended up in Stillwater, MN? Any assistance that you would be willing to offer would be greatly appreciated.

Best Regards, Scott Lovell

Editorial: Climate Change, Continued



A feature article "Energy, Environment and the Future" by Jeff Deschamps in the winter issue of *ACA RefleXions* described practical steps that individuals can take to reduce their personal contributions to greenhouse gases. Judy solicited the article, but we both think that climate change is a subject we should continue to emphasize on the grounds

that scientists are even more concerned about global warming than the general public. In this column I'll try to summarize new developments since the winter issue.

1) There was a very scary article by Elizabeth Kolbert in the Nov. 20th *New Yorker* magazine: "The Darkening Sea." It was the third in a series by Kolbert and they have been collected in her new book, *Field Notes From a Catastrophe: Man, Nature, and Climate Change*, (see the Books Section, page 23). Among other topics, the article discussed "acidification of the ocean" a term coined in 2003 by Ken Caldeira and Michael Wickett, Lawrence Livermore National Lab. The exchange between gases in the atmosphere and those dissolved in water (70% of earth's surface) has become lopsided, with more CO₂ from the air entering the water than coming back out. Bear in mind that the concentration of CO₂ in the air today (380 ppm) is higher than at any time in the last 650,000 years. The sea has absorbed about half of the CO₂ emitted by humans in the last 100 plus years, which is lucky for us because were it not for this great carbon sink we would be in the midst of all the predicted disasters already! However the fact that the other half of the carbon has not yet been absorbed means that even if our CO₂ emissions were stopped completely, tomorrow, the oceans would continue to take up carbon until a new equilibrium is reached.

The seas do have a built-in buffering capacity because if the water's pH starts to drop, shells and shell fragments that have

been deposited on the ocean floor begin to dissolve, pushing the pH back up again. This would be a saving grace except that acidification in our times is not taking place on the same time-scale as deep ocean recirculation. Buffering by ocean sediments is not even a factor in our current situation and paleoceanographers have an example that proves it. 55 million years ago the Paleocene-Eocene Thermal Maximum marked the boundary between epochs by an enormous release of carbon into the atmosphere, possibly from methane hydrate deposits which had been frozen under the ocean floor. This carbon release took place over thousands of years, not mere centuries, and it still happened too fast for the ocean to provide effective buffering.

All that carbonic acid in the sea is already taking a toll; to name just one consequence, coral reefs already suffering from other insults are even more threatened. I encourage anyone wishing to read more about this sobering subject to check out Kolbert's book.

2) On February 2, 2007, the Intergovernmental Panel on Climate Change (IPCC) released "Climate Change 2007: The Physical Science Basis." The report stated that "Average Northern Hemisphere temperatures during the second half of the 20th century were very likely higher than during any other 50-year period in the last 500 years and likely the highest in at least the past 1300 years." that global warming was likely to influence the intensity of tropical storms," and that "Most of the observed increase in globally averaged temperatures since the mid-20th century is very likely due to the observed increase in anthropogenic greenhouse gas concentrations."

The IPCC used 6 different scenarios to model their projections; best estimates for temperature increases by the end of the century ranged from 1.8 to 4°C. and for increase in sea levels from 28 to 43cm. In the estimates for sea level increase, the IPCC had to decide whether or not to include water coming into the oceans as ice caps melt, a process that could have a big impact but is not well understood. They used a conservative approach, with the caveat that: "Models used to date do not include uncertainties in climate-carbon cycle feedback nor do they include the full

effects of changes in ice sheet flow, because a basis in published literature is lacking. The projections include a contribution due to increased ice flow from Greenland and Antarctica at the rates observed for 1993-2003, but these flow rates could increase or decrease in the future." On Feb. 1, 2007 scienceexpress.org published a pertinent article in which an international group (Rahmstorf *et al*) reported that sea level and global mean air temperatures have risen more since 1990 than climate models used in the IPCC predicted. So in fact, the IPCC projection may well underestimate future sea levels.

AAAS President, John Holdren, commented that "The new report powerfully underscores the need for a massive effort to slow the pace of global climatic disruption before intolerable consequences become inevitable." The February 9th issue of *Science* is focused on the problem of energy, in keeping with the theme of the February AAAS meeting. Holdren wrote the *Science* editorial for that issue, on "Energy and Sustainability."

3) In his State of the Union speech President Bush announced plans to address global climate change and energy dependence through a mandatory renewable fuel standard and increased development of solar and wind power. He opposed mandatory caps on carbon emissions, arguing that industry can deal with the problem at less cost by using new technologies. The President's proposals were welcomed by environmentalists, but most think that they fall far short of what is needed to reduce greenhouse gas emissions. The Union of Concerned Scientists warned that the alternative fuels for transport should not include coal-to-liquids. "If alternative fuels are made from coal instead of renewable resources, the president will not meet his stated goal of stopping the projected growth in carbon dioxide emissions from cars, light trucks and SUVs. Instead of cutting global warming pollution, making gasoline or diesel from coal would double the amount of global-warming pollution produced from gasoline today." Philip E. Clapp, President of the National Environmental Trust, commented: "Producing 35 billion gallons of ethanol a year would require putting an additional 129,000 square miles of farmland - an area the size of Kansas and Iowa - into corn production, which is not very likely."

4) Meanwhile, in some quarters, denial that global warming is a problem continues undiminished. On February 3rd, *The Guardian* (London) reported that scientists have been offered cash money to counter the IPCC report. The American Enterprise Institute, an ExxonMobil-funded think tank with close links to the Bush administration, offered scientists and economists \$10,000 each to write articles that emphasize the shortcomings of the UN's IPCC. Travel expenses and additional payments were also offered.

But on a more positive note, on February 15th EnergyBulletin.net reported that "Former Vice President Al Gore and Virgin Group Chairman Sir Richard Branson today announced the Virgin Earth Challenge, a \$25 million global science and technology prize to encourage a technology that will remove at least one billion tons of carbon dioxide equivalent from the atmosphere per year. The prize will be awarded to the individual or group who demonstrate a commercially viable design which will result in the net removal of anthropogenic, atmospheric greenhouse gases each year for at least 10 years without countervailing harmful effects. This removal must have long term effects and contribute materially to the stability of the Earth's climate."

Judy and I hope that readers will be moved to write letters, not only to Congress, but also to us. Perhaps we can stimulate others in our membership to become advocates. Who better qualified than the scientific community to urge our sluggish government to take action?

Connie Chidester

Related websites and some of the sources:

www.ipcc.ch/press/SPM.pdf
www.pewclimate.org/ (Pew Center on Global Climate Change)
www.epa.gov/climatechange/ (Environmental Protection Agency)
www.aaas.org/news/releases/2007/0202ipcc.shtml
www.net.org/warming/sotu.vtml (National Environmental Trust)
RenewableEnergyAccess.com (source for information and news)



Fred Dylla to Head AIP

The Governing Board of the American Institute of Physics (AIP) announced last December the selection of H. Frederick Dylla to be the next Executive Director and CEO of AIP. On April 1, 2007 Dylla replaces Marc H. Brodsky, who held that post at AIP for more than 13 years. Dylla received his B.S., M.S. and Ph.D. in physics from MIT, and has been with the DOE's Jefferson Lab in Newport News, Virginia since 1990, while holding concurrently an Adjunct Professorship in Physics and Applied Science at the College of William and Mary. Dylla is a Fellow and a Past President of the AVS: Science & Technology of Materials, Interfaces, and Processing and is a distinguished lecturer for the society. He is also Fellow of the American Physical Society, and is a founding member of the Forum of Industrial and Applied Physics, currently the largest unit of the APS. He has authored more than 190 publications. With an annual budget of approximately \$75 million, AIP has a staff of 450 employees in its College Park headquarters and its Melville, NY publishing center. More than 134,000 scientists, engineers and educators are represented by AIP through its 10 Member Societies.

2007 Wolf Prize in Chemistry to Ada Yonath



Ada Yonath, the Weizmann Institute, will share the \$100,000 Wolf Foundation Prize in Chemistry with George Feher, UC San Diego. Ada is the Martin S. and Helen Kimmel Professor of Structural Biology; Director, The Helen & Milton A. Kimmelman Center for Biomolecular Structure & Assembly. She was formerly Director of The Joseph & Ceil Mazer Center for Structural Biology, all at the Weizmann Institute of Science. In addition she leads the Ribosome Group in the Weizmann Structural Biology Department. The Wolf Foundation citation states that "The recent emergence of ribosome structures in the crystallographic community is mainly due to Ada Yonath, who uniquely and single-handedly pioneered ribosomal crystallography over more than two decades ago, when others could not even conceive its possibility. By pushing crystallography to its limits, she demonstrated the feasibility of ribosomal crystallography, thus inspiring prominent groups to repeat her experiments. Throughout, she has been the leading force in all stages of structure determination and has introduced fundamental methodological innovations that have greatly impacted the entire field of structural biology." The prize will be presented on May 13 by the president of Israel in the Knesset, home to Israel's Parliament, in Jerusalem.

Merrifield Award to Isabella Karle

The American Peptide Society will present the R. Bruce Merrifield Award for outstanding career achievements in peptide research to Isabella Karle, Laboratory for the Structure of Matter, Naval Research Laboratory, Washington, DC, at the 20th American Peptide Symposium, June, 2007. Their citation stated that "Isabella Karle personally has applied the direct method of phase determination to the pioneering elucidation of molecular formulae and determination of conformations for steroids, alkaloids, frog toxins, photorearrangement products caused by radiation, nanotubes and particularly peptides. For peptides she has established the precise or preferred structures at the atomic level, provided needed parameters for computer drug design programs, useful information for conformation analysis and for synthesizing new analogs with more desirable properties and a basis toward understanding physiological processes." See also the APS Newsletter at americanpeptidesociety.com/publications/newsletter.asp

In her early work at NRL, Isabella developed practical procedures based on the theoretical work developed by her husband Jerome and Herbert Hauptman for the determination of phases directly from the measured intensities of x-ray reflections. These practical procedures have become adopted world-wide and have been essential to the explosive output of crystal structure determinations that are indispensable to the solution of problems in a number of scientific disciplines. She has published more than 380 papers. She was elected to membership in the National Academy of Sciences, the American Academy of Arts and Sciences, and the American Philosophical Society. She has received the Garvan Award of the ACS, the Hillebrand Award, the WISE Lifetime Achievement Award, the Gregori Aminoff Prize, the Bijvoet Medal, the Robert Dexter Conrad Award, and eight honorary doctorate degrees, among them one from the University of Athens (Greece). Isabella was President of the ACA in 1976; at that time the only other woman who had served as ACA President was Elizabeth Wood, in 1957.



Call for Ewald Prize Nominations

The IUCr is pleased to invite nominations for the Ewald Prize for outstanding contributions to the science of crystallography. The Prize is named after Paul P. Ewald in recognition of his significant contributions to the foundations of crystallography and to the founding of the IUCr. The Prize consists of a medal, a certificate and a financial award. It is presented once every three years during the triennial IUCr congresses. Ewald Prize recipients to date are: J.M. Cowley and A.F. Moodie (1987); B.K. Vainshtein (1990); N. Kato (1993); M.G. Rossmann (1996); G.N. Ramachandran (1999); M.M. Woolfson (2002); P. Coppens (2005). The eighth Prize, for which nominations are now being invited, will be presented at the Osaka Congress in August 2008. See <http://www.iucr.org/iucr-top/iucr/invitation08.html> for details about nominations. **The closing date for nominations is 31 August 2007.**

2008 ACA Award Calls

Nominations for the **2008 A. L. Patterson Memorial Award** are due by **May 1st, 2007**. For details see the fall 2006 *ACA Reflexions* or the ACA website: AmerCrystalAssn.org. All nominations should be sent to the ACA office: marcia@hwi.buffalo.edu.

Art in Crystallography Prize

The final deadline for 2007 Prize entries is **May 1st, 2007**. For details see the fall or winter *ACA Reflexions*.



Photo courtesy of Gloria J. Del Bel, HWI

Photos of Marcia and Patti courtesy of Caroline Duax.



ACA's Director of Administrative Services, Marcia Colquhoun (above) and Patti Coley (at right) in their new offices in the amazing new building the Hauptman-Woodward Institute moved to recently, not far from their original location in downtown Buffalo. What a great venue for Herbert Hauptman's 90th Birthday Party (p. 21) and for holding a symposium on Direct Methods in Macromolecular Neutron Diffraction (p.27)

*Please note: 2007 Membership dues can now be paid online.
Also you can register for the Salt Lake City Meeting online.*

NIH Director's New Innovator Awards

Feb. 21, 2007: the NIH announced their **New Innovator Awards**. NIH plans to issue a Request for Applications in mid-March. **The anticipated deadline for application receipts is May 31, 2007.** Applications will be limited to 10 pages, with review and funding for 14 to 16 awards expected by September 30, 2007. **The review will be electronic.** This new program extends the concept of the **Pioneer Awards** to support new investigators of exceptional creativity who propose innovative approaches that have the potential to produce an unusually high impact on significant problems in biomedical and behavioral research. The **New Innovator Awards** will provide grant support to highly innovative new investigators who have not yet obtained a traditional R01 grant. Applicants must hold an independent research position at a domestic institution, and be within 10 years of their terminal degree. The proposed research may be in any scientific area relevant to the mission of NIH (biological, behavioral, clinical, social, physical, chemical, computational, engineering or mathematical sciences). Awards will be made for up to \$300K direct costs per year plus applicable facilities and administrative costs, for five years. It is anticipated that approximately 14-16 awards will be made. For details see grants.nih.gov/grants/guide/notice-files/NOT-OD-07-047.html.

New Name For ACA Website
Please change your bookmarks
to our new domain name:
www.AmerCrystalAssn.org

Please note: VISA Alert

Application procedures for acquiring visas for travel to the US have eased somewhat over the past year. However, the best advice remains to **APPLY EARLY! Applicants are currently advised to apply at least 3 to 4 months in advance.**

There is a very useful website maintained by the International Visitors Office of the National Academy of Sciences: www7.nationalacademics.org/visas/ that answers most questions pertaining to applications for a visa to attend the ACA meeting in Salt Lake City. It also provides links to State Department websites for further information.

Francisco (Paco) Jose Cervantes-Lee: 11/21/1950 - 2/15/2007

Paco Cervantes (B.S., M.S., Universidad de Guanajuato, Mexico; Ph.D. University of Aberdeen, Scotland) was a well-recognized scientist, working in the area of single crystal x-ray structural analysis of small molecules. Subsequent to receiving his Doctorate under the direction of Professor F. P. Glasser he returned to Guanajuato, Mexico and held a post at the University of Guanajuato. In 1986 he accepted an offer to visit the University of Texas at El Paso, initially as a Postdoctoral Fellow working in the general area of organo-transition metal chemistry.

At that time the Chemistry Department at UTEP was involved, along with the Department of Metallurgy, in a major new thrust concerning Materials Science and Engineering funded by the National Science Foundation. Using a combination of grant money and State of Texas funds, the University established a structural facility for the characterization of new materials and metal complexes. Paco agreed to head the new unit of crystal structure analysis. On the basis of his intellectual efforts and technical expertise, coupled with the creative energies of a large number of undergraduate and graduate students, UTEP became well-known as an international center for such activities, and especially for their work on transition metal organometallic systems. Many faculty members at UTEP can directly relate many of their most important scientific results to the excellence of the structural data produced by the Cervantes laboratory.

As a direct result of the recognition accorded the Materials Science and Engineering program, a Ph.D. program in that area was later initiated at UTEP. The success of this degree, the third Ph.D. program at UTEP, was a major reason that other Ph.D. programs were subsequently introduced on campus.

As with all good scientists Paco initiated collaborations outside the region of his base. Significant published work with both



NMSU, Los Alamos National Laboratory and foreign collaborators in Mexico, Russia, Hungary, Romania and England resulted from his research network.

Paco Cervantes was a quiet family-oriented gentleman dedicated to the service of his chosen field. A consummate professional who carried himself with dignity and sincerity, he was, and will always be a model scientist, father and friend. To those of us close to Paco and his family we give thanks to his generosity of time and talent and rejoice in the memory of his childlike joy and happy enthusiasm for those important aspects of his life.

Keith Pannell, U.T. El Paso Department of Chemistry



The photo is from the cover of Brenda Maddox' book "Rosalind Franklin, The Dark Lady Of DNA." For a book review see Physics Today, Feb, 2003, p.61, or the spring, 2003 ACA Newsletter.

Rosalind Franklin Papers

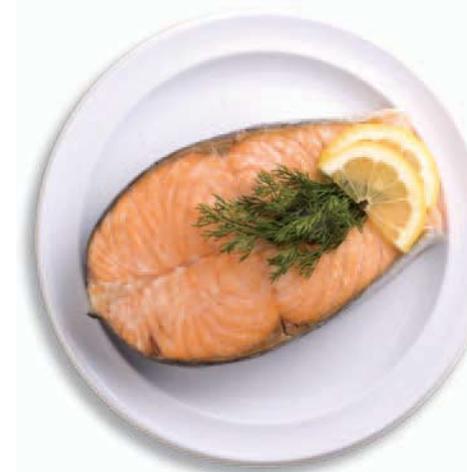
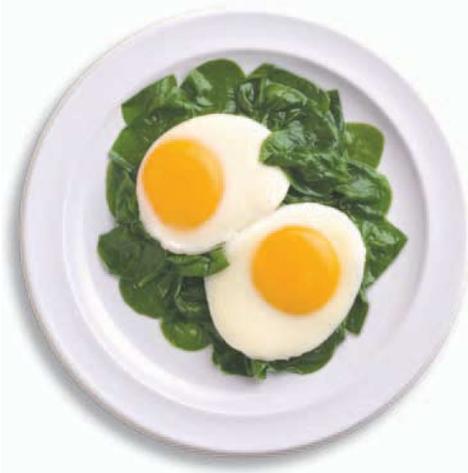
NIH News announced Feb. 6th that the National Library of Medicine has released an extensive selection from the papers of Rosalind Franklin, on its *Profiles in Science* website at <http://www.profiles.nlm.nih.gov>.

Franklin began her scientific career analyzing the structure of coal and carbon during World War II, and became an internationally recognized expert in that field. For five years before her premature death, she did path-breaking research that elucidated the structure of plant viruses. Yet chemist and crystallographer Rosalind Franklin (1920–1958) is now best known for the research that occupied her briefly in between: the structure of DNA.

Early in 1953, when Francis Crick and James Watson were struggling to build an accurate theoretical model of the DNA molecule, it was Franklin's meticulous x-ray diffraction photos and analysis that gave them crucial clues to DNA's structure, and allowed them to win the race for the double helix. Franklin didn't know that there was a race going on, and she never knew that Crick and Watson had access to her then-unpublished data.

Soon after the discovery, Franklin finished her DNA work and moved on to another institution to study viruses. In 1962, four years after her untimely death from ovarian cancer, Crick and Watson received the Nobel Prize for their DNA model, still silent about Franklin's

contributions. Since then she has been recognized and celebrated for her DNA research, even becoming a feminist icon for some. Yet the DNA story often obscures her other brilliant work.



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interfaces with liquid handling robots to speed things up even more. If you're hungry for more information, call 805.681.9009 or visit www.wyatt.com.



ACA COUNCIL OFFICERS - 2007

PRESIDENT

A. Alan Pinkerton
 Dept. of Chemistry
 Univ. of 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
 Univ of Illinois at Chicago
 3100-MBRB
 900 S Ashland Ave
 Chicago IL 60607
 312 413 0339
 Fax: 312 413 9304
bds@uic.edu

VICE PRESIDENT

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

SECRETARY

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

PAST PRESIDENT

Robert Bau
 Dept. of Chemistry
 Univ. of Southern California
 Exposition Blvd.
 Los Angeles, CA 90089
 213-740-2692;
 Fax: 213-740-0930
bau@usc.edu

CANADIAN REPRESENTATIVE

Lee A. Groat
 Earth & Ocean Sciences
 Univ. of British Columbia
 6339 Stores Rd.
 Vancouver, BC
 Canada, V6T 1Z4
 604-822-4525
 Fax: 604-822-6088
lgroat@eos.ubc.ca

APPOINTMENTS

CHIEF FINANCIAL OFFICER

S.N. Rao,
 Max Chambers Library Room 221
 Univ. of Central Oklahoma
 100 N. University Dr.
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 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
 Univ. Estadual de Campinas
 C.P. 6165
 13083-970 Campinas SP, Brazil
 55 19 3788 5497
 Fax: 55 19 3289 3137
torriani@ifi.unicamp.br

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

NEWSLETTER EDITORS

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

Connie Chidester
 2115 Glenwood Dr.
 Kalamazoo, MI 49008
 269-342-1600
 Fax: 716-898-8695
conniechidester@earthlink.net

CANADIAN DIVISION

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

Pawel Grochulski, Secretary
 Canadian Light Source
 Univ. of Saskatchewan
 101 Perimeter Rd
 Saskatoon Saskatchewan
 Canada, S7N 0X4
 306-657-3538
 Fax: 306-657-3535
pawel.grochulski@lightsource.ca

Communications

Cathy Drennan, Chair (04-07)

Dept. of Chemistry
Mass. Inst. Of Technology
77 Massachusetts Ave.
Cambridge, MA 02139
617-253-5622; Fax: 617-258-7847
cdrennan@mit.edu

Annie Heroux (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 Vrieling (07-10)

Univ. of Western Australia
Biomed., Biomolec. & Chem. Sci.
M310, 35 Stirling Highway
Crawley WA 6009
Australia
avrielin@cyllene.uwa.edu.au

Continuing Education

Simon Billinge, Chair (04-07)

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

Gloria Borgstahl (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

Data, Standards & Computing

Ward Smith, Chair (04-07)

Collaborative Access Team
Argonne National Lab.
9700 S Cass Ave. Bldg 436D
Argonne, IL 60439
630-252-0663; Fax: 630-252-0667
wsmith@anl.gov

Bernhard Rupp (05-08)

Biology & Biotech Program L-452
Lawrence Livermore Nat'l Lab
7000 E. Ave.
Livermore, CA 94551
925-209-7429; Fax: 801-880-3982
br@llnl.gov

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)

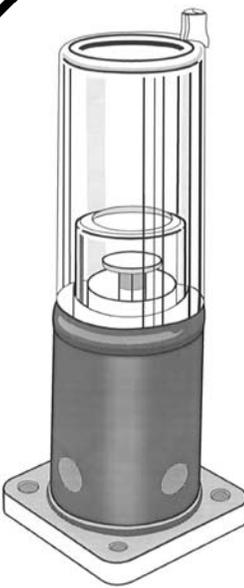
Mat Science & Eng Lab
NIST
Bldg 223 Rm A256
Gaithersburg MD 20899
301 975 5791; Fax: 301 975 5334
winnie.wong-ng@nist.gov

Contributors to This Issue

Alexander Blake, Patti Coley, Marcia Colquhoun, Bryan Craven, Gloria Del Bel, Cathy Drennan, Caroline Duax, Howard Einspahr, Angelo Gavezzotti, Frank Herbstein, Charles Lake, Cora Lind, Scott Lovell, Jason Mathis, Peter Müller, Keith Pannell, Alan Pinkerton, Eric Schramm.

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SPECIAL INTEREST GROUP OFFICERS 2007

Biological Macromolecules**William Royer, Chair, 07**

Dept of Biochem & Mol Pharm.
Univ of Mass Med Sch
364 Planation St
Worcester, MA 01605
508 856 6912; Fax: 508 856 6464
william.royer@umassmed.edu

Carrie Wilmot, Chair Elect, 08

Dept of Biochemistry Mol Bio & Bio-
physics
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 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**Gerald Stubbs, Chair, 07**

Vanderbilt Univ.
Dept. of Bio. Sci.
Box 1820 Station B
Nashville, TN 37235-1820
615 322 2018; Fax: 615 343 6707
gerald.stubbs@vanderbilt.edu

Joseph Orgel, Chair Elect. 08

Dept BCPS
Illinois State Univ Of Tech
3101 S Dearborn
Chicago, IL 60616
312 567 3398; Fax: 312 567 3494
orgel@itt.edu

Amy Kendall, Secretary, 07

Dept. of Biological Sciences
5264 MRB III
Vanderbilt University
Nashville TN 37332
615 322-2012; Fax: 615 343 6707
amy.k.kendall@vanderbilt.edu

General Interest**Peter Mueller, Chair, 07**

Dept. of Chem., MIT
77 Massachusetts Ave Bldg. 2 Rm 325
Cambridge, MA 02139
617 253-1884
pmueller@mit.edu

Allen Oliver, Chair Elect, 08

Dept of Chemistry
Univ of California Santa Cruz
Santa Cruz CA 95064
831 459 2892
alol1@mindspring.com

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, 07**

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, 07

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

Materials Science**Claudia Rawn, Chair, 07**

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

Branton Campbell, Chair Elect, 08

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

Lachlan Cranswick, Past Chair, 07

Canadian Neutron Beam Centre
NRC Canada
Bldg 459, Stn 18, Chalk River Labs
Chalk River, Ontario
Canada, K0J 1J0
613 584 8811 ext 3719
Fax: 613 584 4040
lachlan.cranswick@nrc.gc.ca

Neutron Scattering**Paul Langan, Past Chair 07**

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

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

Powder Diffraction

Thomas Proffen, Chair, 07

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

Cora Lind, Chair Elect, 08

3806 Woodmont Rd
Toledo OH 43613
419 530 1505; Fax: 419 530 4033
cora.lind@utoledo.edu

Claudia Rawn, Sec/Treas 06

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

Service Crystallography

Allen Oliver, Chair, 07

Dept of Chem
Univ Of California, Santa Cruz Santa
Cruz CA 95064
831 459 2892
alol1@mindspring.com

Peter Mueller, Chair Elect, 07

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

Bruce Noll, Secretary, 08

Dept. of Chem. & Biochem.
260B Stephan Hall
Univ. of Notre Dame
Notre Dame, IN 46556
574 631 5935; Fax: 574 613 6652
bnoll@nd.edu

Small Angle Scattering

David Londono, Chair, 07

DuPont Experimental Station
Central Res & Dev
Bldg E323, Rm 109B
Wilmington, DE 19880-0323
302 695 1222; Fax: 302 695 1513
j-david-londono@usa.dupont.com

P. Thiyagarajan, Chair Elect, 07

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

Hirotsugu Tsuruta, Sec/Treas, 07

Stanford Linear Accel Ctr
SSRL/SLAC, MS69
2575 Sand Hill Rd
Menlo Park, CA 94025
650 926 3104; Fax: 650 926 4100
tsuruta@slac.stanford.edu

Alec Sandy, Member at Large, 07

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

Xiaoping Wang, Chair, 07

Dept of Chemistry
Univ of North Texas
Box 305070
Denton TX 76203
940 369 8489
xpwang@unt.edu

Kraig Wheeler, Chair Elect, 07

Dept of Chemistry
Eastern Illinois Univ
600 Lincoln Ave
Charleston IL 61920-3099
cfkaw@eiu.edu

Allen Oliver, Sec/Treas, 07

Dept of Chemistry
Univ of California Santa Cruz
Santa Cruz CA 95064
Tel: 831 459 2892
alol1@mindspring.com

Synchrotron Radiation

James Holton, Chair, 07

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

Richard Gillilan, Chair Elect, 08

MAC CHESS
Cornell Univ
200L Wilson Lab
Ithaca NY 14853
607 255 9386
reg8@cornell.edu

Aina Cohen

SSRL
Stanford Univ
2575 Sand Hill RD MS 99
Menlo Park CA 94025
650 926 3125
acohen@slac.stanford.edu

Young Scientists

Anna Gardberg, Chair, 07

Walters Life Sci M 407
Univ of Tennessee
Knoxville, TN 37996
865 584 5553
agardber@utk.edu

Peter Horanyi, Chair Elect, 08

Biochemistry & Mol Bio
Univ of Georgia
120 Green St
Athens GA 30602
706 461 0534
magyar@virginia.edu

Mark Collins, Secretary, 07-08

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

2007 U.S. NATIONAL COMMITTEE FOR CRYSTALLOGRAPHY

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Innovene USA, LLC
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 A. KANTARDJIEFF (08)**

Dept. of Chemistry and Biochemistry
California State Univ., Fullerton
800 N. State College
Fullerton, CA 92834-9480
714-278-3752; Fax: 714-278-5293
kkantardjjeff@fullerton.edu

Secretary-Treasurer**DOUGLAS OHLENDORF (09)**

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

Members**CHRISTOPHER CAHILL (09)**

George Washington University
Department of Chemistry
725 21st Street NW
Washington, DC 20052
202 994 6959; Fax: 202 994 5873
cahill@gwu.edu

JULIA Y. CHAN (07)

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

PETER KUHN (07)

The Scripps Research Institute
Scripps PARC Institute, CB227
10550 N. Torrey Pines Road
La Jolla, CA 92037
858-784-9114; Fax: 858-784-8996
pkuhn@scripps.edu

CORA LIND (09)

Chemistry Dept.
2262 WO
University of Toledo
419-530-1505; Fax: 419-530-4033
cora.lind@utoledo.edu

JOSEPH NG (09)

Laboratory for Structural Biology
U. Alabama-Huntsville
Huntsville, AL 35899
256-824-3715
ngj@email.uah.edu

MIRIAM ROSSI (07)

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

RONALD E. STENKAMP (07)

Dept. of Biological Structure &
Biomolecular Structure Center
Univ. of Washington
Box 357420
Seattle, WA 98195-7420
206-685-1721; Fax: 206-543-1524
stenkamp@u.washington.edu

CHERYL L. KLEIN STEVENS (08)

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

JENNIFER SWIFT (08)

Georgetown Univ.
Dept. of Chemistry
647 Reiss, 37th and O Streets NW
Washington, DC 20057-1227
202-687-5567; Fax: 202-687-6209
jas2@georgetown.edu

BRIAN H. TOBY (09)

Argonne National Laboratory,
Advanced Photon Source
9700 S. Cass Ave, Bldg. 433/D003
Argonne, IL 60439-4856
630 252-5488
Brian.Toby@ANL.gov

ROBERT VON DREELE (09)

Argonne National Laboratory
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)

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

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WILLIAM DUAX

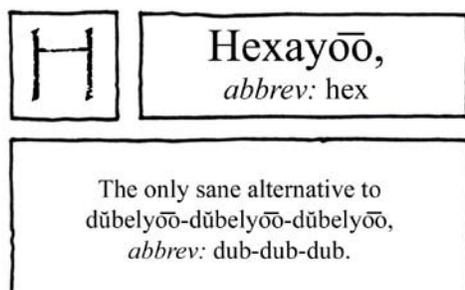
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New Zealand. See:
nearingzero.net/res.html.

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

SCOTT MISTURE
ICDD Representative
Alfred University
misture@alfred.edu

PETER VEKILOV (06)
American Assoc. for Crystal Growth
University of Houston
vekilov@uh.edu

PAUL VOYLES
Microscopy Society of America
University of Wisconsin
voyles@engr.wisc.edu

Ex-Officio Non-Voting Members

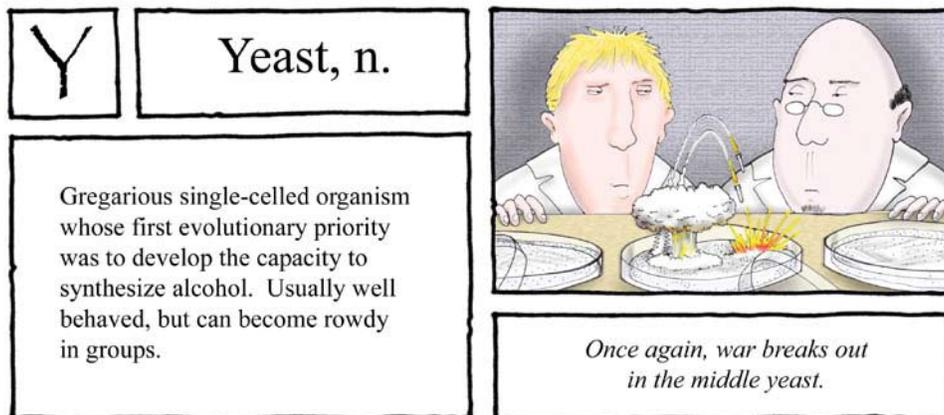
Elsa Riechmanis
(NAS) BCST Co-Chair
Lucent Technologies
er@lucent.com

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

Michael Clegg,
NAS Foreign Secretary
Univ. California at Irvine
mclegg@uci.edu

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

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Isidor Fankuchen (1904–1964) - first President of the ACA

*WL Bragg, Max von Laue and Isidor Fankuchen
(from the Emilio Segrè Visual Archives of the AIP).*

Previous recipients of the Fankuchen Memorial Award in X-ray Crystallography are an illustrious list in the history of the ACA: M.J. Buerger (1971), A. Guinier (1974), Dorothy Hodgkin (1977), D. Harker (1980), L.H. Jensen, (1983), M.G. Rossman (1986), D. Sayre (1989), D.L.D. Caspar (1992), J. Glusker and K. Trueblood (1995), E. Dodson (1998), J.M. Stewart (2001) and A. McPherson (2004) - but who was Fankuchen? I do not remember ever meeting him, but even as a young crystallography graduate student in the early 1950s, I had heard much about "Fan," as he was universally known.

Isidor Fankuchen was born in Brooklyn in 1904, educated locally and then at Cooper Union which is located in the East Village. The school was founded in 1859, and is known for having free tuition and a 13% acceptance rate; www.cooper.edu. Paul Ewald wrote that Fan ran a radio repair shop in Brooklyn to finance his education. His second and third degrees were at Cornell and he then moved to Manchester, England with the support of a Schweinberg Fellowship from Cooper Union. Here he worked with W.L. Bragg; an extension of the Fellowship allowed him to move to the Crystallography Laboratory in Cambridge, then directed by J. D. Bernal, where he obtained a second PhD in 1939.

I have been much intrigued by the question of how Fan (not without Cornell polish) fitted into the somewhat starchy Cambridge atmosphere of the 1930s - a partial answer comes from mentions in Georgina Ferry's biography of Dorothy Hodgkin (*Granta Books*, London, 1998). Fan, described on p. 380 as "the ebullient, enthusiastic American," seems to have been fully accepted, scientifically and socially, in the 1930s club of biological crystallographers. Incidentally, Dorothy Hodgkin made a contribution to the (then recently established) Fankuchen Memorial Fund from her 1964 Nobel Prize money (Ferry, *loc.cit.* p. 239).

Fan accompanied Bernal to Birkbeck College in London at the beginning of the Second World War and only returned to the United States in 1940 or 1941, eventually settling down at Brooklyn Poly (now Polytechnic University) as Professor of Physics, where he remained until his death. It is fair to say that for some years in the 1950s and 1960s Brooklyn Poly was one of the capitals of the crystallographic world, because of Fan, Ewald, Harker, Brill, Post and others. Fan became increasingly involved in administra-

tion and was especially active in spreading the gospel of crystallography through an exhausting schedule of lectures and schools. Ewald called him "the apostle of x-ray diffraction." In addition he was North American Editor of *Acta Crystallographica*, and Ewald estimates that 1500 manuscripts went through his hands between 1948 and 1964. When the American Crystallography Society merged with the American Society for X-Ray and Electron Diffraction to form the ACA, he was elected founding President.

ScienceFinder gives Fan some 80 publications; Ewald mentions a figure of 95. No matter - undoubtedly Fan's glory days in research were the few years he spent in England towards the beginning of the War. Already in 1935 he had published, together with F. C. Bawden, N. W. Pirie and J. D. Bernal, a paper entitled "Liquid crystalline substances from virus-infected plants" (*Nature* (1935), **138**, 1051–1052). The major papers from his stay in England were the steroid study with Hodgkin and Bernal (the magnum opus: "X-ray Crystallography and the Chemistry of the Steroids" *Phil. Trans. Roy. Soc. Lond.* (1940). **A239**, 135–182.) and three consecutive papers on plant viruses with Bernal, "Structure of the Particles, Biological Implications: I. X-ray and Crystallographic Studies of Plant Virus Preparations; II. Introduction and Preparation of Specimens; III. Modes of Aggregation of the Virus Particles," in *J. Gen. Physiol.* (1941). **25**, 111–120; 120–146; 147–165. These papers were very influential - the steroid study showed that the Wieland-Wiand formula for steroids, which had led *inter alia* to Nobel Prizes in Chemistry in 1927 and 1928, could not be correct, while the virus study showed that viruses were crystalline as well as having liquid crystalline properties. Thus, structure determination of viruses by diffraction methods was feasible (as we well know now).

However, return to America was more or less the end of a chapter for Fan. As part of the war effort he worked on the abortive Habbabuk project, the attempt to build enormous aircraft landing platforms constructed from sea ice and wood shavings (see M. F. Perutz, "I wish I had made you angry earlier", *OUP*, New

Biographical Sketch of Fankuchen, cont'd

York, (2002)). Establishing Brooklyn Poly as a leading crystallographic center took most of his energy, and he returned to biological crystallography only a few times in the 1940-1960 period. His students and coworkers pioneered structure determinations at low temperatures, mostly on substances liquid at room temperature. Monochromators remained an interest, stimulated originally by the need to obtain high-intensity monochromatic radiation for the virus studies. And there were many studies to map out the capabilities of diffraction methods in studying reactions in the solid state and applications to dentistry. In this way many new areas were opened up but a grand theme like that of the English period was not established. "To everything there is a season, and a time to every purpose under the sun," *Ecclesiastes* 3:1.

Acknowledgements: I have not found a biography of Fan but P. P. Ewald published an obituary in *Acta Cryst.* (1953), 17, 1091-1093. There is also a legendary but unpublished memoir by Ben Post that I have not succeeded in tracking down. Two of Fan's students followed in his footsteps and became Presidents of the ACA—the late Ben Post (in 1966, may his memory be blessed) and Hugo Steinfink (in 1995, may his years be multiplied).

To Hugo, many thanks for your help.

Frank Herbstein.



Isidor Fankuchen talking with playwright Arthur Miller and artist Joel Tobias. The History of Science Mural at the Polytechnic Institute of Brooklyn is in the background.

(from the Emilio Segrè Visual Archives of the AIP)

On the Cover: 2007 Trueblood and Fankuchen Awards

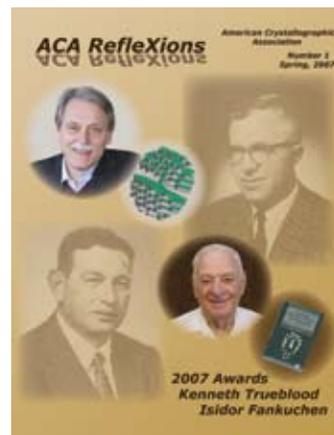
Angelo Gavezzotti (Professor, Dipartimento di Chimica Strutturale e Stereochimica Inorganica, U. Milano), will receive the 2007 Kenneth N. Trueblood Award, and Frank Herbstein, (Professor, Dept. of Chemistry, Technion-Israel Inst. of Technology, Haifa), will receive the 2007 Isidor Fankuchen Award at the annual ACA Meeting July 21-26 in Salt Lake City. Their award lectures will be presented at special symposia which have been organized in their honor.

Angelo is at top left with an image of a spherical cluster (split up to show the molecular arrangement inside), from the crystal structure of 1,2-dicyanobenzene (J.Janczak,R.Kubiak, *Acta Cryst.* **C51**, 1399, 1995) showing the extreme polarity of the structure (space group Pmn2₁, z vertical). The coordinates were generated using Angelo's program ATTACH for the calculation of surface tension coefficients. The graphic program used was SCHAKAL, by E.Keller (Freiburg). See the Books section, page 22 for a description of Angelo's IUCr monograph, just published.

Frank Herbstein is at lower right with an image of Vol 1 of his two volume encyclopedic work: *Crystalline Molecular Complexes and Compounds*, Oxford University Press, 2006, (an IUCr Monograph on Crystallography).

Both Fankuchen and Trueblood are both former ACA Presidents, in 1950 and 1961, respectively. The originals of the photos of Kenneth Trueblood (above right) and Isidor Fankuchen (below left, courtesy of Patti Coley) are stored in the Niels Bohr Library of the American Institute of Physics, and are in the Roster of Presidents in *Crystallography in North America*, Eds. Dan McLachlan, Jr., and Jenny P. Glusker; published by the ACA in 1983.

Editor's note: See the biographical sketch of Isidor Fankuchen by Frank Herbstein that precedes this.



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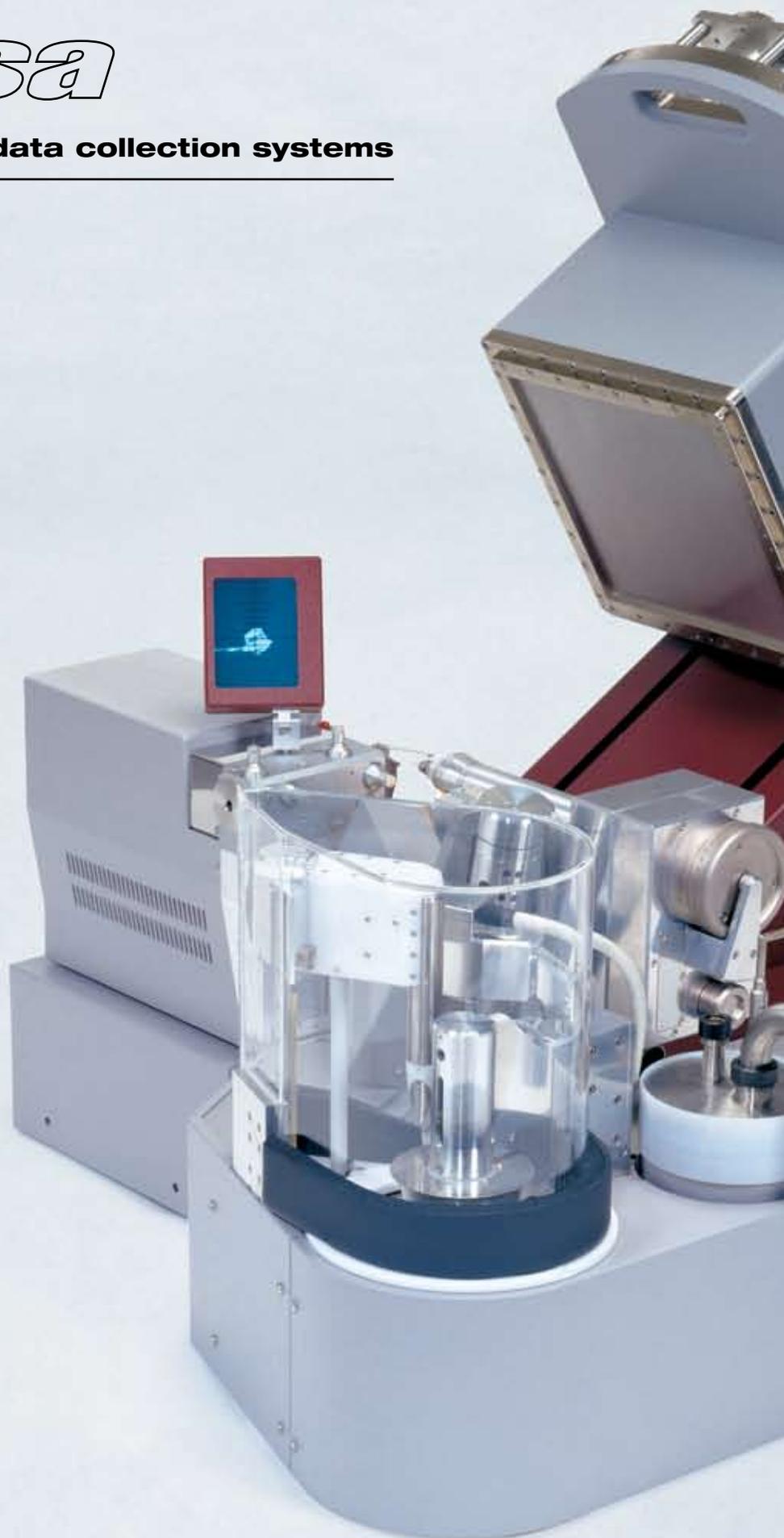
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Web Watch: Members of the Communications Committee of the ACA encourage everyone to participate in the Crystallography Web Watch Column. The web address of web sites of interest to crystallographers and a brief description should be sent to Cathy Drennan at cdrennan@mit.edu. Thank you in advance for any suggestions.

Crystallography Teaching: web-based basic course on crystallography: escher.epfl.ch/eCrystallography/

Cool crystal movies (e.g. watch izit dye soak into lysozyme crystals): ruppweb.org/level1/movies_list.htm

Phase diagrams: www-structmed.cimr.cam.ac.uk/Course/Crystals/Theory/phases.html

Analyzing crystallization trials: xray.bmc.uu.se/~terese/crystallization/library.html

Anti-Science / Intelligent Design News

News abstracted from the National Center for Science Education (NCSE: www.ncseweb.org)

On Feb. 13, 2007, the Kansas state board of education voted 6-4 to approve a set of state science education standards in which evolution is treated in a scientifically appropriate and pedagogically responsible way. They tossed out the standards adopted in November, 2005 which had been severely criticized by the NAS, the AAAS and the National Science Teachers Association as tainted with creationist ideology including a definition of science aimed at allowing supernatural explanations for natural phenomena. This reversal was a direct consequence of the 2006 elections when several board members sympathetic to intelligent design failed to win re-election.

Feb 14th: The **2006 AAAS Award for Scientific Freedom and Responsibility** was awarded to the executive director of the NCSE along with nine science teachers who have been on the front lines of the battle to prevent introduction of intelligent design into science classrooms as an alternative to evolution. Eight of the teachers fought efforts by the Dover Area District School Board in Pennsylvania to require the reading of an anti-evolution statement in 9th grade biology classes; the other, as head of the science department at North Cobb High School in Kennesaw, Georgia, took on a public role in opposing a decision by the Cobb County School Board to require stickers on biology textbooks that read, in part: "Evolution is a theory, not a fact, regarding the origin of living things."

February 3rd, *Le Monde* reported that thousands of copies of *The Atlas of Creation*, by the Turkish creationist Harun Yahya,

were recently sent to French schools, colleges, and universities. The "richly illustrated" 770-page book purports to show "the secret links between Darwinism and bloody ideologies like fascism and communism." It also contains a photograph of the 9/11/01 attacks on the World Trade Center, with a "stupefying legend" blaming terrorism on "Darwinism" and calling it the "only ideology that valorizes, and therefore encourages, conflict." The French minister of education promptly directed academic administrators not to distribute the book. The article noted that the mass distribution of unsolicited creationist literature in France is reminiscent of recent incidents in the UK and New Zealand, where Christian creationist organizations sent packets of anti-evolution material, including DVDs, to government schools.

From the *Los Angeles Times*, Feb. 12th, 2007: Edward Humes, author of *Monkey Girl: Evolution, Education, Religion and the Battle for America's Soul* (see Books section, page 20), commemorated Darwin Day by addressing the pervasive misunderstanding of evolution by the public. "There are really two theories of evolution," he said. "There is the genuine scientific theory, and there is the talk-radio pretend version, designed not to enlighten but to deceive and enrage. The purveyors of "the awful and pervasive straw-man image of evolution" are all too effective, Humes lamented. Not only did Judge Jones, who presided over the *Kitzmiller v. Dover* case, receive death threats after his decision, but also "teachers across the nation tell me they feel compelled to downplay or skip evolution lessons to avoid controversy; one L.A. area high school instructor said she is the only one of five science teachers on her faculty to even mention evolution in class, notwithstanding a clear state mandate to teach it."

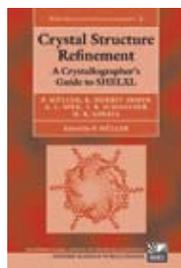


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A celebration of Herbert Hauptman's 90th birthday and of science (!) was held February 14th at the Hauptman-Woodward Institute in Buffalo. Herb and his great-neice Michelle Heller are at center left. Clockwise from top right: Dick Griffin in the background and Herb talking with Peter Ostrow, the MC of the proceedings; Steve Potter at left with Bob Blessing and his daughter Marlene; David Langs talking with Chris Gilmore; Davide Viterbo and his wife Mariella. Photos are courtesy of Caroline Duax.

Crystal Structure Refinement – A Crystallographer’s Guide to SHELXL, (IUCr Texts on Crystallography 8), Peter Müller (ed), Oxford Univ. Press, (2006), hardcover, 232 pp, \$98.50, ISBN: 0-19-857076-7.



Peter Müller first studied crystallography with George Sheldrick at the University

Reviewed by Alexander (Sandy) Blake. Sandy is Principal Research Officer and Manager of the Crystal Structure Service of the Chemistry Dept. at U. Nottingham, UK. He is also Deputy Validation Editor, and a Co-Editor of *Acta Crystallographica*.

of Göttingen, Germany and later worked in the Department of Molecular Biology at UCLA. Since 2004 he has been Director of the X-ray Facility in the Department of Chemistry at MIT. His interests include low temperature data collection methods and data collection strategies. He has given many conference presentations on the practice and teaching of crystallography.

Along with his four co-authors he has produced an excellent book describing the features and use of *SHELXL*. By a wide margin *SHELXL* is the most popular program for the refinement of small molecule structures, and it is one of the top three programs for the refinement of macromolecular structures.

But why do you need this book when you already have the *SHELXL* manual that came with the program? Well, not only does the book expand in great detail on topics that are covered only briefly in the manual, but it also covers other topics that lie outside the scope of a program manual. For example, while the manual has about five pages on twinning, this book devotes no fewer than 44 to the topic, and valuable chapters explore in detail important matters such as atom type assignment and structure validation that are not covered in the manual. In fact, these topics are often not covered at all in books on structure determination, and certainly not in the depth achieved here.

As well as the arguably more obvious chapters on refinement, the treatment of hydrogen atoms, disorder, twinning and structure validation, the book also covers *SHELXL* program organization, atom type assignment, pseudosymmetry and crystallographic artefacts, and there is a chapter on miscellaneous topics. For macromolecular crystallographers there are chapters on protein refinement and validation. The book also offers a foreword by George Sheldrick that contains a short history of the origin and evolution of *SHELXL*, as well as an overview of the program.

There is a wealth of practical advice for the refinement of both routine and difficult structures, and topics are well illustrated by the use of examples and case studies: the relevant *SHELXL* .INS and .HKL files are supplied on CD, so that the reader can carry out the refinements described in the text. To drive home the point that this book and the *SHELXL* manual are complementary, the CD also includes a copy of the manual.

Molecular Aggregation: Structure Analysis and Molecular Simulation of Crystals and Liquids (IUCr Monographs on Crystallography)

by Angelo Gavezzotti, Oxford Univ. Press, (2007), hardcover, 384 pp, \$130.00, ISBN: 198570805

Angelo Gavezzotti is the 2007 Trueblood Award recipient. (see cover and page 17). Part I of the book provides a brief but accurate summary of all the basic ideas, theories, methods, and conspicuous results of structure analysis and molecular modelling of the condensed phases of organic compounds, that is: quantum chemistry, the intermolecular potential, force field and molecular dynamics methods, structural correlation, and thermodynamics. It is written in simple and intuitive form so that the reader may easily find the essential background for the discussions in the second part. Part II discusses the present status of studies in the analysis, categorization, prediction and control, at a molecular level, of intermolecular interactions in liquids, solutions, mesophases, and crystals. The main focus here is on the links between energies, structures, and chemical or physical properties. Jack Dunitz commented: “Fills a gap in the market ..., original and very topical, touching on the areas of molecular structure analysis, applied quantum theory, intermolecular forces, molecular dynamics, all with emphasis on the condensed states of matter.” *From the book description in Amazon.com.*



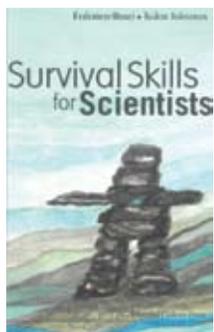
Monkey Girl: Evolution, Education, Religion, and the Battle for America’s Soul, by Edward Humes,

Ecco, (2007), hardcover, 400 pp. \$17.10, ISBN-10: 0060885483

Edward Humes is a Pulitzer Prize-winning journalist who researched the case in Pennsylvania, *Kitzmiller et al. v. Dover Area School District* that came to trial before Judge John E. Jones III in the fall of 2005. The media billed the trial as a replay of the 1925 Scopes Monkey Trial. Humes' title is taken from the taunt leveled at a child whose mother objected to the new policy. Humes manages to convey the intensity and drama of the trial atmosphere. Told from the perspectives of all sides of the battle, *Monkey Girl* is about what happens when science and religion collide. Some parents, including teachers in the school district, viewed intelligent design as a stealth form of creation science. Although many of these parents were Christians (two even taught Sunday school), they felt that teaching ID in a public school classroom improperly injected religion into education. In Judge Jones' eloquent ruling for the plaintiffs, he noted: “This case came to us as the result of the activism of an ill-informed faction on a school board, aided by a national public interest law firm eager to find a constitutional test case on ID, who in combination drove the Board to adopt an imprudent and ultimately unconstitutional policy.” The citizens of Dover had reached a verdict in a school board election earlier - they ousted every one of the 8 incumbents who favored ID.



Survival Skills for Scientists by **Federico Rosei** and **Tudor Johnston**, Imperial College Press (August 2006), hardcover: 205 pages \$38.00, ISBN: 1860946402; paperback, 205 pp. (Sept., 2006), ISBN: 1860946410.

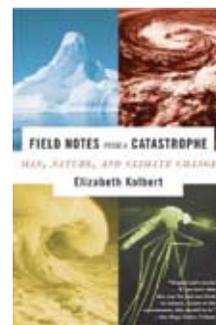


There are not many books designed to help a young scientist make the hard choices while transitioning from undergraduate to graduate studies, then post-doctoral

fellowships and finally real jobs; most must rely on advice of mentors or more experienced friends. The discussions of careers in academia, industry and government labs, in the US and elsewhere, are reputed to be amusing and easy to read. See the review in *Science*, **314**, 24th Nov., 2006, p 1245, by D.F. Perepichka.

Field Notes from a Catastrophe: Man, Nature, and Climate Change, by **Elizabeth Kolbert**, Bloomsbury USA, hardcover: (March, 2006), 192 pp. \$18.36, ISBN: 1596911255; paperback: (December, 2006), 240 pp., \$11.16, ISBN: 1596911301.

Expanding her three-part *New Yorker* series, journalist Elizabeth Kolbert examines the immediate and far-reaching consequences of global warming, calmly letting facts tell the story. She also discusses the contentious political debate on this issue, chiding the U.S. government for refusing to sign on to the Kyoto Accord. The book is not unrelentingly pessimistic; in one chapter she singles out Burlington, Vt., for its impressive energy-saving campaign, which ought to be a model for the rest of the nation.



The First Scientific American: Benjamin Franklin and the Pursuit of Genius, by **Joyce Chaplin**, Perseus Books Group; 352 pp., hardcover, (2006), \$21.73, ISBN: 0465009557; paperback, (April 2007), \$13.75, ISBN: 0465009565.

In this biography, Harvard historian Joyce Chaplin has made Franklin's scientific career her main focus. Although his early experiments with electricity were sensational, Franklin had to make his fortune before he could become accepted into the international Enlightenment science establishment. Chaplin describes how he crafted his public image as a scientist to transform himself from a humble colonial tradesman into a sophisticated gentleman of letters, then goes on to tell about the areas of science that attracted Franklin in his forties and fifties. See the review in *Science*, **315**, 9th Feb. 2007, p 768 by H. Frederick Dylla.



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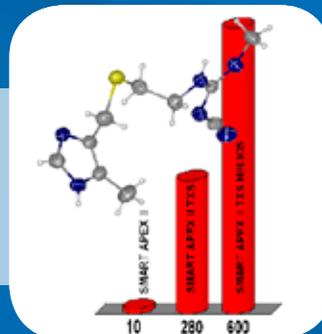
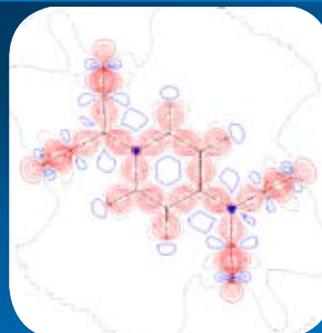
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Crystallography

Bruker/MIT Symposium

The symposium, held February 9-11, 2007, at MIT, was hosted by the Dept. of Chemistry, organized by the Director of the departmental X-Ray Diffraction Facility **Peter Müller**, and sponsored by Bruker-AXS. The theme of the symposium was *Extreme Diffraction Data - the Cutting Edge of Structure Determination* and speakers kept to this theme with talks on charge density calculations and time-resolved x-ray diffraction studies. **Sue Byram** (Bruker-AXS) opened the meeting, introducing the latest hardware developments. **Gregory Petsko** (Brandeis), showed examples of time-resolved x-ray crystallography in his presentation "Structural Enzymology in Four Dimensions." Petsko described how he is using Laue-diffraction methods to collect several complete data sets from the same crystal within a few milliseconds and stressed the importance of in-house x-ray sources for any kind of time-resolved work. In his presentation "APEX2 ULTRA – Precision and Accuracy," **Michael Ruf** (Bruker-AXS) introduced one of the latest developments of his company. This instrument combines the brightest Mo-radiation source currently available with the APEX2, a CCD detector that has low noise and very high dynamic range, thus creating a setup ideal for charge density work. **Tibor Koritsanszky** (Middle Tennessee State U.), is one of the leading figures in the international charge density community and co-author of the refinement program XD. His talk "X-Ray Charge Density Methods" gave an overview over the theory behind charge density calculations and helped the audience to better understand the potential but also the limitations of this method.

The lunch break was combined with a poster exhibition. An independent jury awarded the best poster with a \$500 prize. This year, the jury was headed by **Marilyn Olmstead** (UC Davis), and the **2007 Bruker/MIT Poster Prize** went to **Paula Piccoli** (Argonne National Laboratory) for her poster "Neutron Diffraction and X-Ray Charge Density Studies of



From left: Philip Coppens, Christopher Cummins, Dietmar Stalke, Sue Byram, Tibor Koritsanszky, Peter Müller, Louis Farrugia, Michael Ruf, Paula Piccoli.

Tetraacetylene." **Dietmar Stalke** (U. Göttingen) asked: "What Can a Synthetic Chemist Learn from Charge Density?" Stalke presented impressive results of charge density analyses from his ongoing research. **Christopher Cummins** (MIT) talked about "Synthetic Cycles for Small Molecule Activation, Atom Transfer, and Reactive Metal Complex Regeneration," describing how members of his research group were able to chemically activate elemental group 15 molecules to yield organic nitriles from N₂ and a variety of unusual P-containing ligands directly from P₄. **Louis Farrugia** (U. of Glasgow) is well known to most chemical crystallographers for his programs (for example WinGX and the Platon taskbar) but is also a pioneer in charge density methods. Touching on one of the biggest challenges in the field of x-ray charge density calculations, he described the "Difficulties in the Topological Characterization of Bonds to Transition Metals." The final speaker of the symposium was **Philip Coppens** (SUNY Buffalo). Coppens is a leading researcher both in the world of charge density and in the field of time-resolved studies. His presentation on "Time-Resolved Diffraction and the Evaluation of Charge and Spin Densities of Molecular Excited States" was a brilliant finale, combining the two major themes of the symposium in one fascinating talk.

Coupled to the symposium was a two-day charge density refinement workshop focusing on the use of the program XD to analyze ultra-high resolution data and to derive and visualize deformation density, electrostatic potentials, bond critical points and other important molecular properties. Thirty-two geographically diverse participants attended. **Farrugia** and **Koritsanszky** were joined in the teaching by **Anatoly Volkov** and **Philip Coppens** from SUNY Buffalo, so students benefited from the experience of four of the world's foremost figures in the charge density scene.

The Bruker/MIT Symposium has been held every year since 1995, except 2003, and has grown in recent years. This year's symposium was the most international one yet and resulted in several new dialogs between scientists and even in two rather concrete plans for collaborations. The preparations for the 2008 Bruker/MIT Symposium have already begun (the date has yet to be determined).

Peter Müller



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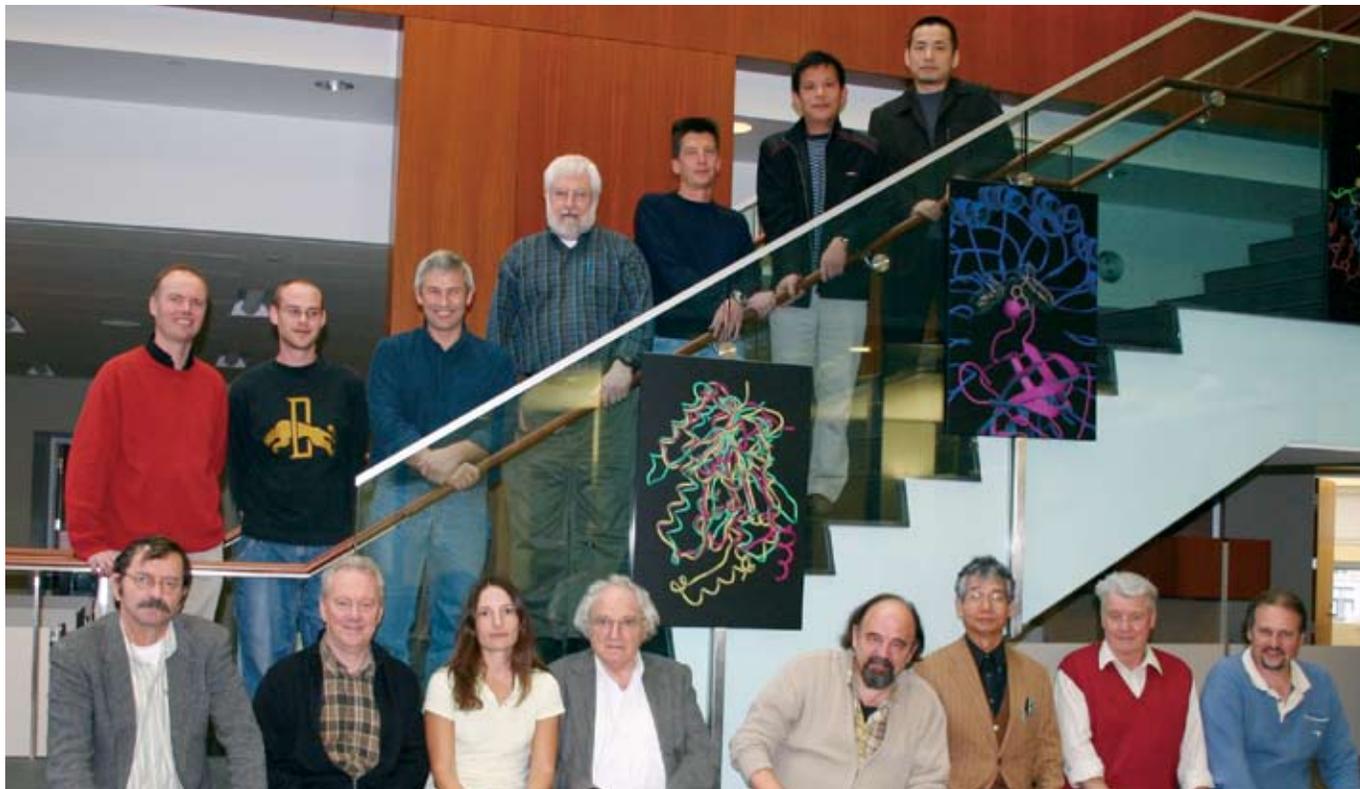


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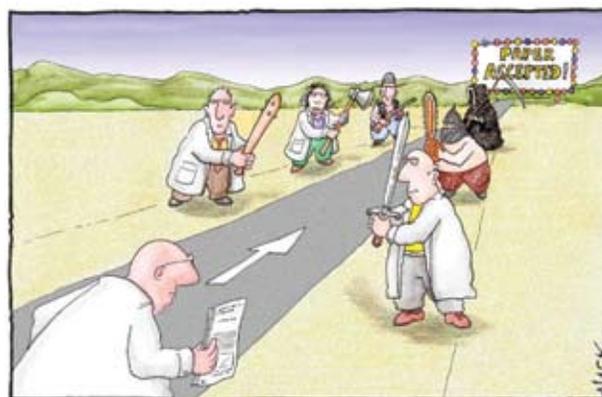
Top row, l to r: Eddie Snell, Matthew Blakeley, Dean Myles, Robert Blessing, Andreas Ostermann, Hongliang Xu and Kazuo Kurihara; bottom row, David Langs, Peter Timmins, Flora Meilleur, Herbert Hauptman, Alberto Podjarny, Nobuo Niimura, Andre Mitschler and Michael Haertlein. Photo courtesy of Gloria J. Del Bel, HWI.

A kickoff symposium on *Direct Methods in Macromolecular Neutron Diffraction* was held at the Hauptman-Woodward Medical Research Institute in Buffalo on October 16, 2006. In spite of Buffalo's widely publicized and debilitating "surprise" October storm, symposium speakers and participants from the United States, France and Japan gathered at HWI to present the latest developments in neutron crystallography, exchange new ideas and plan future collaborative research activities. The two-day meeting was held in connection with the grant that Herbert A Hauptman, HWI President and Nobel Laureate, received from The Human Frontier

Science Program Organization to support his ground-breaking research project entitled *New Methods of Biomolecular Crystal Structure Determination Specific to Neutron Diffraction Data*. which will be a collaborative effort among scientists in the US, France and Japan over the next three years. Hauptman opened the symposium with a lecture on direct methods in neutron crystallography. Ten other speakers also gave lectures on key topics, ranging from neutron diffraction studies and experiments on fully-deuterated proteins to neutron diffraction facilities and measurements, and neutron direct methods and phase determination.

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by Nick D. Kim, U. Waikato, New Zealand.
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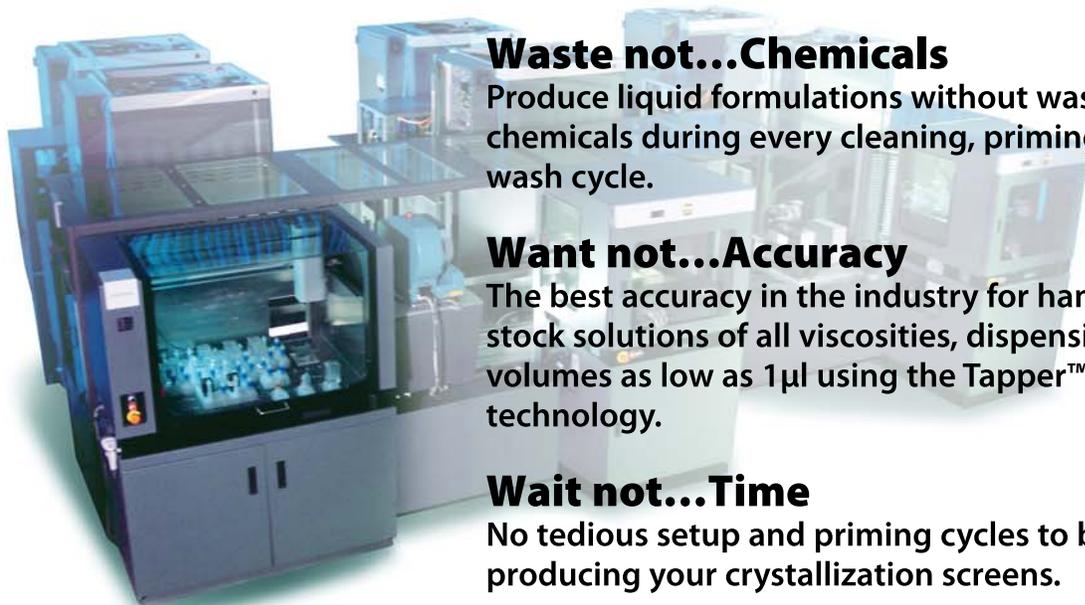


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The ACA Summer Course in Small Molecule Crystallography, 2007

This course will be offered at the Indiana University of Pennsylvania (IUP) campus from July 9th through July 18th, 2007. IUP is located in the town of Indiana, PA about 80 miles east of Pittsburgh. A van service will be provided to and from the Pittsburgh Airport on Sunday July 8th and Wednesday July 18th. Each day there will be three lectures in the morning on single crystal and powder diffraction methods, followed by afternoon and evening workshops and computer tutorials covering topics ranging from problem solving to crystal structure determination. Attendees are encouraged to bring their own single crystal or powder samples for x-ray data collection and are expected to have at least an undergraduate science degree (we have had successful students from biology, chemistry, geoscience, physics and materials science). No prior experience of x-ray crystallography will be assumed, but attendees are advised to read in advance *Crystal Structure Analysis: A Primer*, by Jenny P. Glusker and Kenneth N. Trueblood, Oxford Univ. Press (1985).

The organizers aim for a total of 25 attendees, who in past years have come from academia (students and faculty), and from government and corporate institutions, both in the U.S. and from abroad. We encourage applications from Latin America. Tuition and board (single occupancy, including breakfast and lunch) will be \$650 (\$1000 for those from Corporate Laboratories).

Instruments available on site will be three Bruker-Nonius diffractometers (a CAD4 and D8 Advance at IUP and an APEX II instrument with CCD detector located at Duquesne University electronically linked to the Lab at IUP). In previous years, Rigaku and Bruker have set-up state-of-the-art instrumentation for use during the course including

Summer School Faculty:

Jennifer Aitken, Duquesne U. *Solid-state chemistry, powder diffraction.*

Nattamai Bhuvanesh, Texas A & M. *Solid-state chemistry, powder diffraction.*

Robert Blessing, HWI & SUNY, Buffalo. *Structural biol., Shake n Bake.*

Bryan Craven, IUP. (Course co-organizer). *Crystallography, charge density, neutron diffraction.*

David Duchamp, formerly Pharmacia, Kalamazoo, MI. *Structures of small biomolecules, crystallographic software.*

Steven Geib, U. Pittsburgh. *Service crystallography of small molecules.*

Jenny Glusker, Inst. for Cancer Research-Fox Chase, Philadelphia, *Structure solution, structural biology*

Curt Haltiwanger, Cephalon, Inc., West Chester, PA. *Single crystal diffraction and structure determination.*

James Kaduk, Innovene USA, Naperville, IL. *Crystal structure determination from powder diffraction.*

Wim Klooster, Australian Nuclear Sci. and Tech. Org., *Single Crystal Neutron Diffraction*

Charles Lake, IUP. (Course co-organizer). *Inorganic structures, crystallographic teaching.*

Peter Mueller, MIT. *Service crystallography of small molecules.*

Hamilton Napolitano, Universidade Estadual de Goias, Brazil. *Structures of small bioorganic molecules.*

Robert Stewart, Carnegie-Mellon U., Pittsburgh. *Theory of X-ray scattering, charge density studies*

Brian Toby, Argonne National Lab. *Neutron Diffraction, Powder Structure Determination.*

Brian Wargo, Freedom High School, Pittsburgh & graduate student U. of Pittsburgh. *Powder diffraction tutor.*

John Woolcock, IUP. *Inorganic structures from crystallography and nmr.*

a Rigaku Miniflex powder diffractometer, Rigaku SPIDER and SCXmini benchtop single crystal instruments and a Bruker APEX II single crystal instrument. The computer labs will have ample space and each attendee will have access to an individual computer. The computers will have access to the Bruker and Rigaku versions of *SHELX*, the Cambridge structural data base, *GSAS/EXPGUI* and the **Crystmol** software packages.

The course registration form can be obtained from the ACA website: www.AmerCrystAssn.org. Completed forms must be received before June 1st, 2007 by Bryan Craven, Chemistry Dept, Indiana Univ. of Pennsylvania, Indiana, PA 15705, USA (or sent electronically to Charles H. Lake at lake@iup.edu). Further information can be obtained from craven@icubed.com or lake@iup.edu; also see aca.hwi.buffalo.edu/ACA2007SummerCourse.html.

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

Bryan M. Craven and Charles H. Lake, Organizers



BSR2007 will bring together the world's leading authorities in the biological applications of synchrotron radiation for a four day program, which will include lectures by leading academics including: Janos Hajdu (Uppsala U.), Shigeyuki Yokoyama (RIKEN Genomic Sciences Centre), Sir Tom Blundell (U. Cambridge), Keith Hodgson (Stanford U.), Nobel Laureates Johann Deisenhofer (Howard Hughes Medical Institute), Hartmut Michel (Max Planck Inst. Biophys) and, (to be confirmed) Roger Kornberg (Stanford).

The academic program is available online at www.bsr2007.com. The program includes plenary lectures, academic sessions and networking opportunities. Join us to learn about the latest advances in the field and have an opportunity to visit the Diamond Light Source in Oxford, one of two new major synchrotron facilities opening in Europe.

The deadline for abstract submission is June 30, 2007.

The conference will take place at the Bridgewater Hall, Manchester, UK on 13th-17th August 2007; Conference Chairs are **Samar Hasnain** and **Louise Johnson**.

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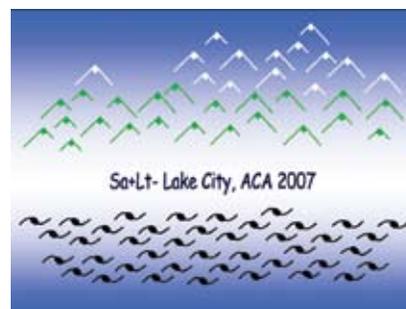
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**ACA 2007 July 21 – 26 Salt Palace Convention Center,
Salt Lake City Utah**

Advance Registration Deadline: June 1, 2007
Advance Hotel Registration Deadline: June 13, 2007
 Register online and see Call for Papers online at
www.AmerCrystalAssn.org



PROGRAM CHAIR:
Jill Trehwella
jtrehwella@usyd.edu.au
 Fax 61 2 935 147 26
 Phone 61 2 935 187 82



LOCAL CHAIRS

Chris Hill
 801-585-5536
chris@biochem.utah.edu
 Fax 801-581-7959

Heidi Schubert
 801-585-9776
heidi@biochem.utah.edu
 Fax 801-581-7959

Workshops, Saturday, July 21st

Full Day - **SHELX** – Refinement of Twins/Disorder and Phasing with **SHELX, C,D,E**
Part 1: Refinement of Disordered, Twinned and High-Resolution Structures (Small and Macromolecules).
Part 2: Experimental Phasing of Macromolecules.
Speakers: George Sheldrick, Regine Herbst-Irmer, Peter Müller, Thomas R. Schneider, Ton Spek

Half Day -Standards for Publication of Macromolecular NMR Structures

Award Symposia

Kenneth N. Trueblood Award in honor of Angelo Gavezzotti
Isidor Fankuchen Award in honor of Frank Herbstein
 Margaret C. Etter Early Career Award in honor of Cora Lind

The Elizabeth A Wood science writing award will be presented to
 Lisa Randall at the Awards Banquet July 25th.



Transactions Symposium

Diffuse Scattering for the Masses: Local Structural Correlations in Molecular, Macromolecular, and Inorganic Crystals
Speakers: Ross Angel, Simon Billinge, James Britten, Branton J. Campbell, Donald Caspar, Friedrich Frey, Lars Meinhold, George N. Phillips, Lee Robertson, Stephan Rosenkranz, T.Richard Welberry



Spiral Jetty, North end of the Great Salt Lake



Antelope Island (Photos by Eric Schramm).



2007 Nobel Laureate **Roger Kornberg** has accepted Local Chair Chris Hill's invitation to speak. He will give the first talk in the BIOMAC *Large and Difficult Structures* session the morning of July 26th.

Registration fees

Fee	Advance (before June 1)	Late (after June 1)
Regular Member	\$390	\$585
Retired Member	\$156	\$234
Post doc Member	\$195	\$293
Student Member	\$156	\$234
Nonmember*	\$585	\$878
Post doc Nonmember*	\$293	\$439
Student Nonmember*	\$234	\$351
Guest**	\$ 50	\$ 50

SHELX Workshop – full day **\$110 (60 students)**
SHELX Workshop – half day **\$70 (40 students)**

Mentor/Mentee Dinner

Mentor	\$30
Mentee	\$20
Banquet	\$55 (\$25 students)

*The nonmember registration fee includes a complimentary membership to the Association for 2007. Those registering as nonmember post docs or nonmember students must include documentation of this status with registration form.

**Guest registration includes Opening Reception, Exhibit Show and Get Together on Sunday morning.

Register on-line or download forms to register by fax or by mail.

www.AmerCrystalAssn.org
 Questions: aca@hwi.buffalo.edu



*Above: Fly Fishing on the Provo River
 Photo by Eric Schramm*

*Below: Salt Lake Skyline, with Oquirrh Mountains
 Photo by Jason Mathis*

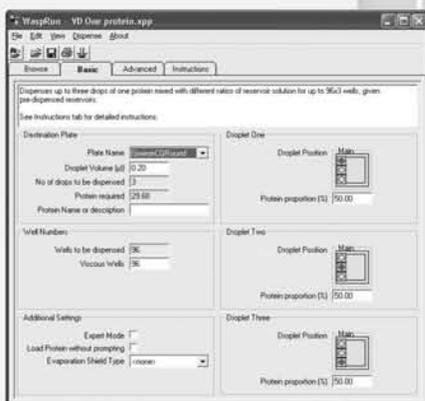
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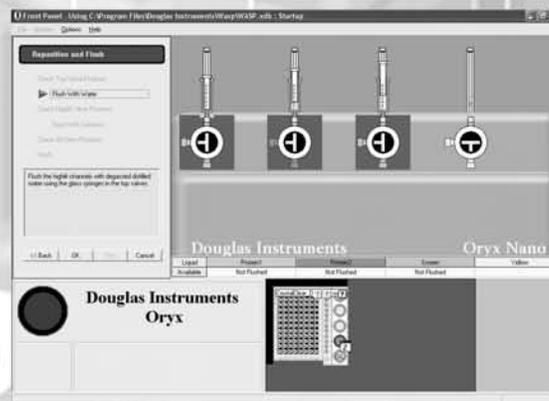


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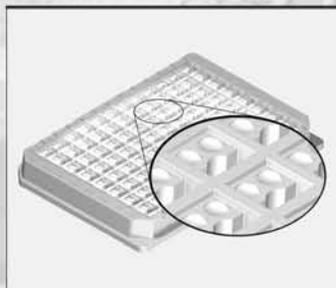


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Biological Macromolecules

New Structures
 Strategies for Crystallization Challenged Macromolecules
 Experimental Phasing with Longer Wavelength X-rays
 New Membrane Protein Structures
 Informatics in Structural Biology
 Function from Structure: *Janet Thornton, Doug Brutlag, Sung-Hou Kim, Osnat Herzberg, Aled Edwards, Alfonso Valencia*
 Computational Methods
 Large and Difficult Structures: *Venki Ramakrishnan*

Industrial

Impact of Crystallography in Industry: *Barry Finzel, John Barker, Ping Chen, Giovanna Scapin*

Materials Science

Non-Ambient Crystallography
 Mineralogy and Crystallography: Real Crystals, Extreme Conditions: *Bryan Chakoumakos, Lee Groat, George Lager, Ron Peterson*

Neutron

Neutron Macromolecular Crystallography
Julian C.-H. Chen

Powder Diffraction

SDPD (Structure Determination from Powder Diffraction): *Getting Better and Better!* *Abraham Clearfield, Carmelo Giacovazzo, Chris Gilmore, William I.F. David, Jason P. Hodges, James Kaduk, Peter W. Stephens, Robert Von-Dreele, Matthew Peterson*

Small Angle Scattering

USAXS/USANS: *Dale Schaefer, Paul Butler, Godarajan Muralidharan, Andrew Allen*
 Characterization of Surfaces and Interfaces: *Changyong Park, Randall E. Winans*
 X-ray Imaging and Resonant Scattering

Small Molecules

Important Science from Small Molecule Structures
Bruce Foxman, Joel Miller, Chick Wilson
 Tricks of the Trade: Interpretation of Structural Results
Larry Falvello, Anthony Spek, Phillip Fanwick, Victor Young
 Supramolecular Chemistry
Christer Aakeröy, Len Barbour, Silas Blackstock, Kenneth Doxsee, Bruce Bart Kahr, John MacDonald
 Cool Structures

Young Scientist

FLYS – Fun Lectures for Young Scientists
 Undergraduate Research Showcase

Joint Symposia

General Interest I and II

Advances in Data Collection
 Detectors: *Mark Tate, Gerard Bricogne*
 Biomacromolecular Assemblies and Biomembranes
B.T. Nixon, J.K. Krueger, H.W. Huang, J.G. Grossmann, S. Krueger, J. Lipfert
 Time and Field Dependent Responses in Scattering Experiments: *Wim Pyckhout-Hintzen, Charles Dewhurst, Tom Mason, Matthew Kramer, Jim Richardson, Jon Hanson*
 Structural Mechanisms of Infectious Disease
 Energy Storage and Conversion
 Nanostructures
 Micro-Crystals, Micro-Beams, and Multiple Crystals
 Teaching Gadgets and Educational Tools: *Wally Cordes, Jenny Glusker, Henk Schenk*
 Radiation Damage

Exhibit Show 2007

The exhibition is scheduled to begin on the evening of Saturday, July 21 in conjunction with the Opening Reception. The 2007 Show will run through Wednesday, July 25. The Advertising and Exhibits Div. of the AIP is managing the show. For further information contact Bob Finnegan, AIP, 2 Huntington Quadrangle, Suite 1N01, Melville, NY 11747, rfinneg@aip.org, ph. (516) 576-2433; fax (516) 576-2481.

JUNE 2007

7-17 **Engineering of Crystalline Materials Properties: State-of-the-Art in Modeling, Design, and Applications**, the 39th crystallographic course at the Ettore Majorana Centre, Erice, Italy. www.crystalerice.org/Erice2007/2007.htm.

JULY 2007

1-6 **Gordon Research Conference on Electron Distribution and Chemical Bonding**, Mount Holyoke College, South Hadley, MA. Carlo Gatti, Chair; Dylan Jayatilaka, Vice-Chair.

11-13 **Neutrons in Biology**, Oxfordshire, UK. www.isis.rl.ac.uk/conferences/nib2007/

9-18 **ACA Summer School in Small Molecule Crystallography**, Indiana University of PA, craven@icubed.com or lake@iup.edu.

21-26 **ACA Annual Meeting - Salt Lake**



City, Utah. **Local Chairs:** *Chris Hill* (U of Utah, chris@biochem.utah.edu) & *Heidi Schubert* (U of Utah, heidi@biochem.utah.edu), **Program Chair:** *Jill Trehwella* (Univ. of Sydney), b2jtrehwella@usyd.edu.au.

JULY 2007

29-8 **Small-Molecule Crystallography Summer School**, San Diego, CA. Arnold L. Rheingold, arheingold@ucsd.edu; <http://chem-tech.ucsd.edu/Recharges/SMXF/crystalschool.html>.

AUGUST 2007

13-17 **BSR2007: 9th International Conference on Biology and Synchrotron Radiation**, Manchester, UK. www.srs.ac.uk/bsr2007/.

22-27 **ECM-24** Marrakech, Morocco. www.ecm24.org.



SEPTEMBER 2007

3-6 **Advanced Methods in X-Ray Charge Density Analysis**, Martina Franca, Italy. piero.macchi@unimi.it, nicola.casati@istm.cnr.it, simona.galli@uninsubria.it.

NOVEMBER 2007

4-7 **AsCA-Asian Crystallographic Association Meeting**, Taipei, Taiwan R.O.C. www.asca2007.tw/index.html

MAY 2008

31-June 5 **ACA Annual Meeting -Knoxville, TN** **Local Chair:** *Jason Hodges* (SNS Division - ORNL, hodges@ornl.gov). **Program Chair:** *Paul Butler* (NIST, butler@nist.gov).

AUGUST 2008

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



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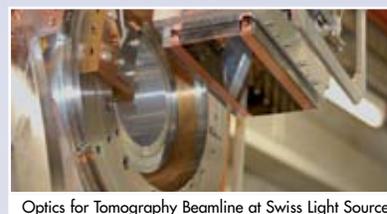
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- References: ANL, CLS, Desy, Jenoptik, PSI, Carl Zeiss Laser Optics

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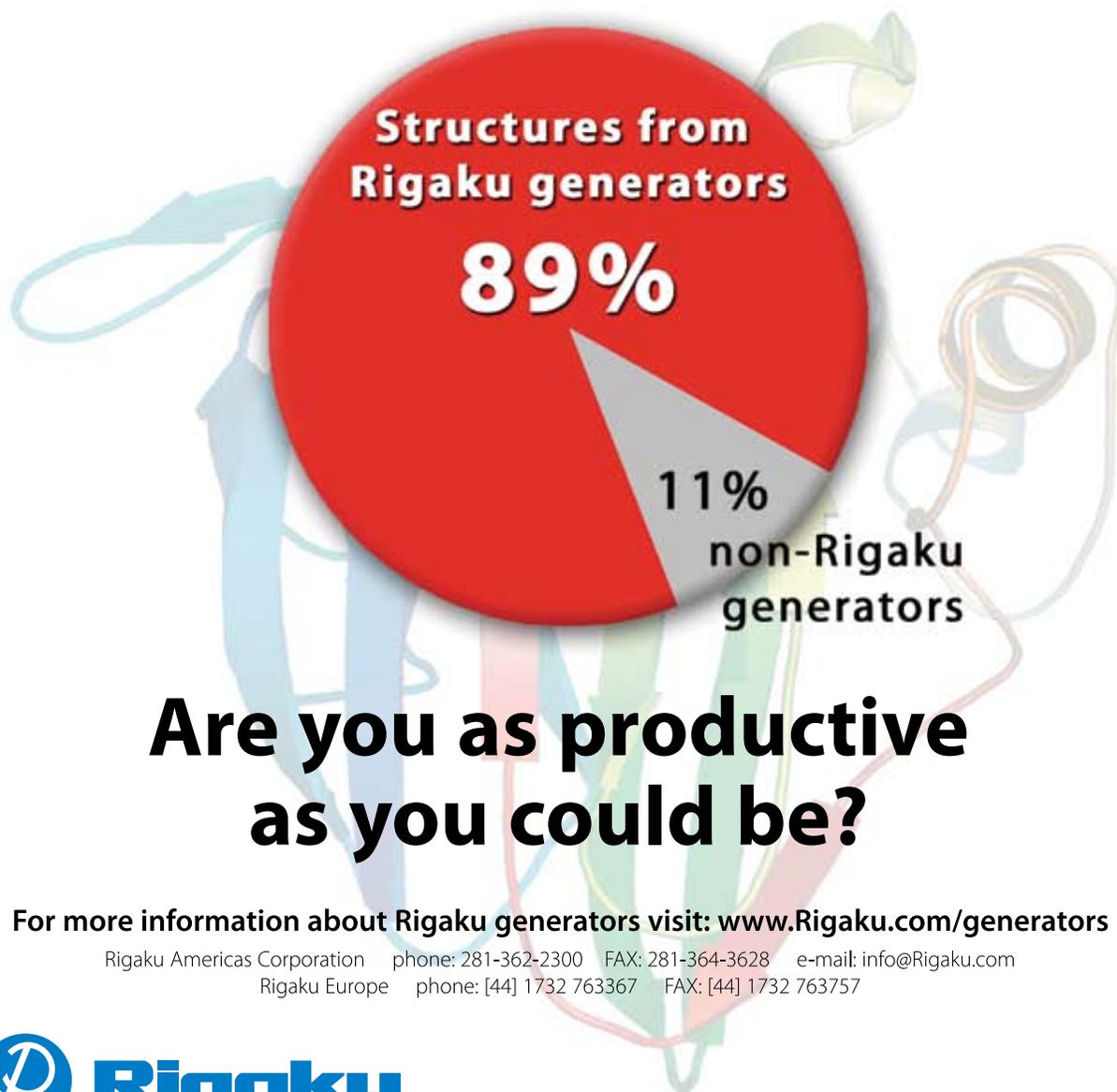
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