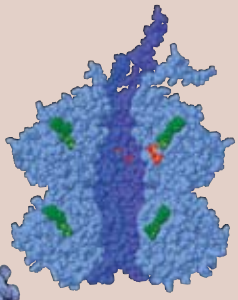
ACA RefleXions

AMERICAN CRYSTALLOGRAPHIC ASSOCIATION

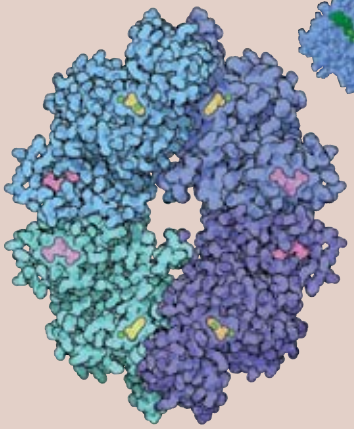
Number 2

Summer 2008

$$U_H^2 \leq \frac{1}{2}(1 + U_{2H})$$



$$n\lambda = 2d \sin\theta$$

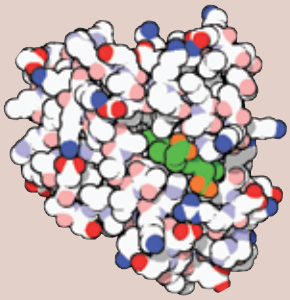


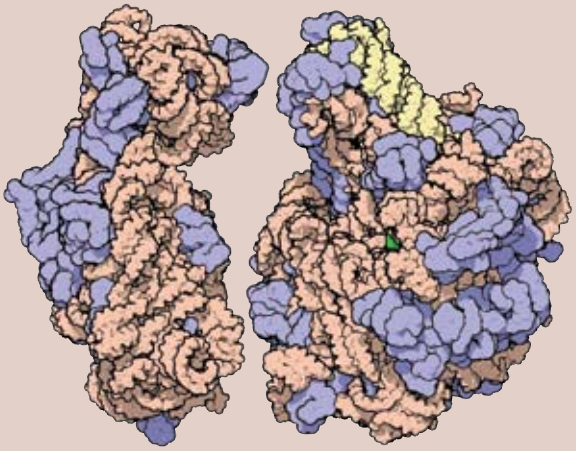
$$R = \frac{\sum ||F^o| - |F^c||}{\sum |F^o|}$$

$$F_H = \theta_H \sum_K F_K F_{H_K}$$

$$\tan\phi_H = \frac{\sum_K |E_K E_{H-K}| \sin(\phi_K + \phi_{H-K})}{\sum_K |E_K E_{H-K}| \cos(\phi_K + \phi_{H-K})}$$

$$P(u, v, w) = \sum_{hkl} |F^o_{hkl}|^2 e^{-2\pi i(hu+kv+lw)}$$





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ACA RefleXions

American Crystallographic Association

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

Table of Contents

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

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Things move fast in an IUCr year. The Knoxville ACA meeting opened the weekend after Memorial Day with four workshops, over 30 exhibitors and 650 registrants. The meeting attracted a number of scientists from around the world. We were especially honored to have Yuji Ohashi, President of the IUCr, as well as Chris Gilmore and Iris Torriani from the IUCr Executive Committee with us in Knoxville. Tennessee is the "*volunteer state*", and we owe the success of the Knoxville meeting to the many volunteers who helped with our annual meeting, but a special thank you goes out to Program Co-Chairs Paul Butler and Dean Myles, our SIG Chairs who coordinated many of the sessions, and Local Chair Jason Hodges, and their hard working committees. Thanks also to Marcia Colquhoun and her ACA staff; Patti Coley, Jen Shepard and new hire Crystal Towns for all that they do to make our organization successful throughout the year, especially at the annual meeting.

We will present a more complete coverage of the Knoxville meeting and its scientific program in the fall issue of *RefleXions*, but I will summarize a few of the highlights while it is still fresh on our minds. One highlight of the meeting came Sunday evening, June 1st, when nearly 350 attendees had the opportunity to take a field trip to ORNL to tour new ultra-high-intensity (1.4MW) Spallation Neutron Source. Special thanks to Al Ekkebus and the folks at ORNL for their hospitality and for being such gracious hosts and tour guides. The *Transactions* Symposium on "*Complementary Methods to Crystallographic Techniques for Structure/Function studies of Biological Macromolecules*" organized by Carrie Wilmot and Susan Krueger featured lectures on the complementary use of spectroscopy, neutron diffraction, SAXS and NMR to study structure. The *Transactions* Symposium was particularly appropriate for a meeting near ORNL and was well attended.

Other highlights included our award presentations. The Margaret C. Etter Early Career Award that seeks to "recognize outstanding achievement and exceptional potential in crystallographic research demonstrated by a scientist at an early stage of their independent career." The 2008 **Etter Award** was presented to **Radu Custelcean**, Research Staff Member at ORNL recognizing his creative research in crystal engineering of novel and functional metal organic framework structures for selective ion binding. The A. L. Patterson Award that seeks "to recognize and encourage outstanding research in the structure of matter by diffraction methods, including significant contributions to the methodology of structure determination and/or innovative application of diffraction methods and/or elucidation of biological, chemical, geological or physical phenomena using new structural information." The 2008 ACA **Patterson Award** was presented to ***Bi-Cheng (B.C.) Wang*** for his "significant contribution to the methodology of structure determination from single isomorphous replacement or single-wavelength anomalous scattering data and for its impact on structural biology". The *BioMac SIG* organized a session in B.C.'s honor on Wednesday, June 4th, featuring talks by B.C., Wayne Hendrickson (the first Patterson Awardee) and others. In attendance were several members of B.C.'s family, including three grandchildren!

Your ACA Council members were busy with two full days of meetings before the ACA meeting and working lunches every day of the meeting. The ACA Council met on Friday before the meeting to review final preparations for the Knoxville meeting and the finances of the ACA, and to finalize plans for the meeting and banquet. A number of ACA policy issues were discussed. Council voted to post its minutes on our website, so it will now be easier for members to track Council actions. During the week we met with the SIG chairs and future program and local chairs to monitor the status of preparations for upcoming meetings (July 25-30, 2009; Toronto / July 24-29, 2010; Chicago / May 28 – June 2, 2011; New Orleans and July 21-26, 2012, Boston).

On Saturday before the meeting we met with the USNCCr where the main topic was preparations for IUCr Congress in Osaka this August 23-31. I will take this opportunity to congratulate **David Sayre** who will be presented with the **8th Ewald Prize** at the Opening Ceremony in Osaka. I also will remind our members of the **ACA Summer School on Small Molecule Crystallography being held** July 7-16 at the Indiana University of Pennsylvania. 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.

This is an election year. The Democrats have finally settled on their nominee. Thanks in large part to Louis Delbaere, the ACA nominating committee has a full slate of candidates ready for our annual elections this fall. My thanks and congratulations go out to Winnie Wong-Ng and Judith Kelly for running for Vice-President, and to Patrick Loll and Carrie Wilmot who are running for Secretary. You can find more information about them and our other candidates in this issue of *RefleXions* (pages 22-33).

Finally, on behalf of the ACA Council and our membership, I want to thank Alan Pinkerton for his past service as ACA President and memorable "a cappella talking blues" tribute to reciprocal space at the ACA banquet. I encourage members to contact me, or any of your Council representatives, with your ideas for improving the operation of the ACA or our annual meetings.

I hope to see you many of you at the IUCr meeting in Osaka this August.

Marv Hackert

To the Editors:

When reading the announcement for the annual meeting I noticed that the ACA hopes to make this year's meeting 'carbon neutral'. The ACA should be applauded for this effort. While this is a step in the right direction that should help raise everyone's awareness of the problem of global warming I hope it is not the end point.

Being carbon neutral refers to neutral (meaning zero) net carbon release. This is accomplished by balancing the amount of carbon released with an amount sequestered or offset (i.e. carbon offsets). The ACA will accomplish this purchasing carbon offsets (or encouraging attendees to purchase such offsets) from ***CarbonFund.org.*** This is where the ideal begins to break down. There has been considerable criticism of carbon offsets. It is important to remember that a carbon offset is merely a financial instrument representing a reduction in net greenhouse gas emissions. This is not a real reduction in emissions, just an attempt to remediate some or all of those emissions through projects that sequester carbon dioxide or pay others to reduce their emissions by an amount that offsets your emissions. Offsets have also been criticized because they are difficult to verify (due to their indirect nature) and there are no standards for the companies providing these offsets. While some providers obtain independent certification that their offsets are accurately measured, the credibility of the various certification providers has also been questioned. Some disagree with the principle of carbon offsets and complain they are merely a mechanism for assuaging guilt rather than real changes in behavior. Environmentalist and writer George Monbiot says that carbon offsets are an excuse for business as usual with regards to pollution (see: *"Selling Indulgences"* originally published in the *Guardian, October 18, 2006,* available online at ***www.monbiot.com/archives/2006/10/19/selling-indulgences/***).

If carbon offsets are not the solution what is? When speaking with an energy planner in a local government she made a very pertinent observation… "the best kilowatt hour is the one never used". This means that the first and most effective action we can all take is to reduce our power consumption. This provides a real decrease in carbon emissions, not the 'net decrease' offsets provide. After reducing our demand for power as much as possible through conservation we can look at other means of reducing our "carbon foot-print". One alternative to offsets (supported by the Izaak Walton League) is a market-based measure, such as cap-and-trade. This policy places caps on emissions and companies would need to either reduce their emissions to comply with the cap or buy excess reductions from another company better situated to reduce their own emissions. Unlike offsets this results in real reductions in emissions because the cap is set to an amount lower than current emission levels. Another alternative available in some locales is to purchase power generated through renewable resources such as solar, wind, or hydroelectric. It is probably too late for the ACA to request power generated from renewable resources but this is something to keep in mind when planning future meetings.

Jeff Deschamps

Notes from the AIP Meetings 26-28 March 2008

The American Institute of Physics Executive Committee, Governing Board and the Assembly of Scientific Society Officers met at the American Center for Physics in College Park. The AIP is evolving under the leadership of the new Chief Executive Officer, Fred Dylla. One of the most visible new directions is a weekly newsletter, *AIP Matters,* with information on current activities on a broad spectrum of publishing and public policy issues. *AIP Matters* is e-mailed to AIP Board and Staff, but a web interface is being set up at ***www.aip.org/*** to allow others interested to sign onto the mailing list. It's really worth a look. Another periodic email called FYI, from the Physics Resources Center, provides up to date information concerning the status of legislative and public interest initiatives on Capitol Hill. FYI is available to anyone interested and to subscribe simply go to ***www.aip.org/fyi/***. Both distributions are interesting and useful.

CEO Dylla reported to the Governing Board on several activities. He has been active in meeting challenges posed by new Open Access laws, which also had been a priority for his predecessor, Marc Brodsky. Notable is the mandate written into the 2008 Consolidated Appropriations Act on behalf of the NIH and its Library of Medicine (PubMed). The new law makes voluntary submission mandatory for all NIH-supported publications stating: ***"the NIH shall implement the public access policy in a manner consistent with copyright law."*** NIH has precluded substantive discussion with representatives of publishing organizations until very recently, when a pro-forma discussion was held on very short notice. Dylla represented the AIP at this brainstorming session. Elias Zerhouni (Director of NIH) appeared favorably impressed by his presentation.

The NIH position places the entire burden of compliance on individual PIs, who must thread a rather narrow path between non-compliance and violations of copyright law, and who have the least coherent legal representation. This lack of clarity in implementation appears to be an intentional effort by NIH to dilute responsibility for compliance as much as possible and, to blunt efforts of publishing organizations to preserve the value added by peer review and copy editing . A curious response to this situation has developed at Harvard University, where some have begun their own web-mounting of pdf files. Skirmishes probably will remain interesting for some time to come. It is important for PIs to learn how each publishing house will implement compliance with NIH policy. AIP journals allow authors to mount peer reviewed manuscripts on both institutional and personal websites, similar to the Harvard policy, while they do not allow third party commercial use without express permission. The American Chemical Society volunteers to deposit manuscripts on behalf of authors. AIP is considering making deposits directly to Pub Med Central for NIH funded investigators, in line with ACS practice

Another innovation is to devote some of each Governing Board meeting to general scientific presentations. Robert Socolow's talk was one of these; the other was given by Kevin Marvel, of the American Astronomical Society on eight landmark discoveries of 2008. His talk was punctuated with clever nicknames for most of the discoveries.

Little science actually penetrates the legislative process. Several of CEO Dylla's efforts are directed at changing this situation. Among the more important and generally applicable is his suggestion that we all contact our own representatives and simply ask them if they have scientific advisors. If not, as will often be the case, VOLUNTEER! Dylla's activities also include a growing relationship with Steve Israel, Congressman from the Long Island district where AIP publications are located. Congressman Israel has responded positively to a tutorial organized by Dylla, which brought in four experts in the area of climate change and sustainable energy.

Two high level retirements marked the turn of the year. Darlene Walters announced her retirement as Sr. Vice President for Publishing. She will leave as soon as a replacement has been appointed. Darlene prevailed over the many challenges posed by online publishing, and the enterprise is now stronger than it has been at any time during her tenure. Jim Stith had previously announced his intention to retire after his tenth year as Vice President, Physics Resources Center, discussed further below. Jim and Darlene will be hard to replace and we wish both well!

Stith's tenure has been marked by important policy and public education initiatives. Among the most visible of these are programs administered by Alicia Torres, as part of the Media and Government Relations division. Discoveries and Breakthroughs Inside Science (DBIS; ***www.aip.org/dbis/***) provides 30 second spots on scientific progress in a variety of areas. Initially funded by the NSF, this program is slowly becoming self-supporting. Its signal importance is that it reaches a much larger audience than do programs like NOVA, which are viewed primarily by folks who already know something about science. DBIS actually reaches a younger, broader, and far less scientifically literate audience. Statistical metrics indicate, moreover, that it is remarkably effective at raising scientific consciousness. The Inside Science News Service (ISNS: ***www.aip.org/isns/)*** presents similar types of coverage aimed at scientific journalists, rather than at the general public. It is a rather brilliant source of "instant" text on scientific "current affairs." A detailed example if ISNS stories involved the adaptation of breathalyzer technology to measure concentrations of ~10^3 medically important compounds and the use of such data in compiling detailed spectra of an individual's health status. Both the DBIS and the ISNS services are entering a period of what appears to be sustained growth, and they illustrate the excitement in the Physics Resources Center.

A telling statistic described by Jim Dawson (ISNS) is that approximately the same percentages (~35%) of the population read scientific stories as read the sports pages. Given this parity, it is hard to understand why science awareness falls so short. A continuing focus of the PRC is to understand how to encode scientific ideas and data into media that facilitate decoding by the intended audiences. Macromolecular crystallographers should be aware that Jason Bardi (***jbardi@aip.org***), one of the writers for ISNS, is formerly a graduate student of Cynthia Wolberger.

Alicia Torres and Jason Bardi will discuss their Media activities with the ACA Council in Knoxville. Among the possibilities are preparation of key new results from submitted abstracts for the purpose of advertising the meeting. A related suggestion: implemented by the Acoustical Society among others, is to have an online news room promoting their national meeting.

The Media and Government Relations Center (MGR) is also monitoring the distribution of a new film produced by Ben Stein called "Expelled". This film presents itself as a cogent public interest film addressing academic freedom for proponents of Intelligent Design. I've not seen the film, but its promotion has been lavish and hard to identify with the creationist movement (see page 10).

A final note on the MGR activities concerns the Campaign Education Workshop, that was held on 10 May 2008 to educate potential candidates for political office about the ins and outs of running campaigns. As the perennial need for scientific training in our elected representatives has never been greater, this presents an appropriate opportunity io improve the situation.

Excellent presentations at the Assembly of Scientific Society Officers were grouped around four topics: evolution of new algorithms for using the internet and Open Access publishing implications; federal funding levels and what can be done now, workforce and career development in the physical sciences, and how AIP and member societies can capitalize on opportunities in energy and climate research. It was of more than passing interest that Francis Slakey (APS) holds the distinction of being the only human to have surfed the major surfing beaches AND climbed the highest peaks on on all continents! His talk on chipping away at the carbon footprint one technology wedge at a time was a terrific seque to a talk during the Governing Board meeting the next day by Robert Socolow of Princeton University, who is the author of the wedge strategy. Although these presentations made much creative use of numbers, it appears that California has achieved what could be argued as a carbon neutral economy for an extended period since their efforts began in the 1970s. This put into fine perspective the intense fears promulgated by many that dealing with the greenhouse gases will necessarily harm "the economy". The twin problems of climate change and sustainable energy have clearly emerged as an important AIP priority, and they are seeking to enlist member societies in their search for solutions.

Charlie Carter

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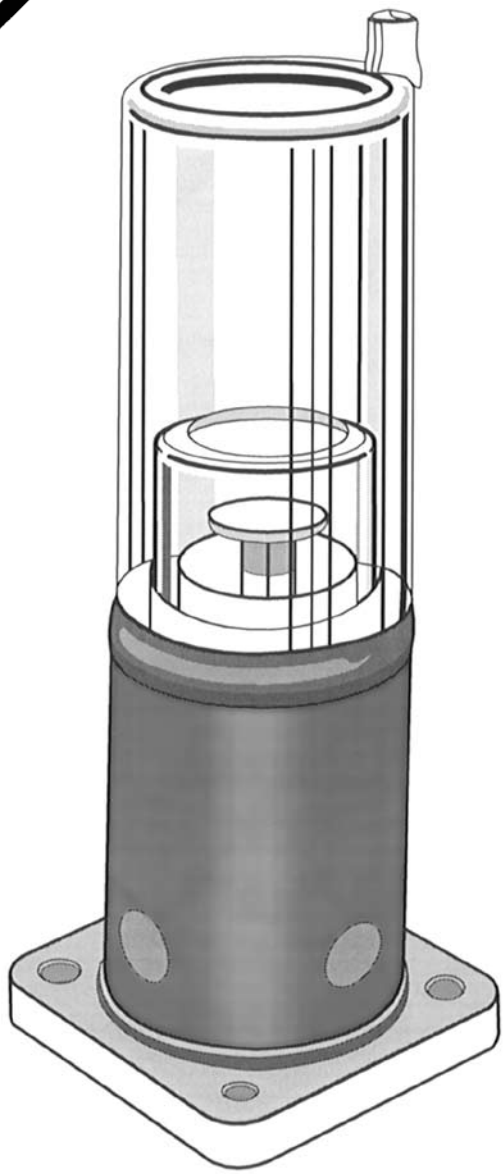

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News from Canada

The Larry Calvert Travel Award is presented by the Canadian National Committee for Crystallography to assist students in attending the IUCr Congress. This year support for travel to Osaka has been awarded to ***Daniel Lee*** and ***Jimin Zheng*** from Queen's University and ***Nobuhiko Watanabe*** from the University of Alberta. Congratulations!

Chemical and Materials Diffraction at the CLS (Saskatoon): The Brockhouse Sector for Materials Diffraction and Scattering has been funded and will provide three simultaneous beamlines for powder, small molecule, and scattering experiments. It should be coming on line in 2011. In the meantime, a diffractometer is being commissioned at the Hard X-ray Micro-Analysis (**HXMA**) beamline at **CLS 06ID-1.** This a multipurpose hard x-ray beamline, based on a 63 pole superconducting wiggler. The HXMA has been designed to provide the community with XAFS, K-B mirror microprobe, and x-ray diffraction (including non-ambient) capabilities. A CCD detector being ordered.

More details can be found at ***www.lightsource.ca/experimental/hxma.php*** or contact ***Chang-Yong Kim*** at (306) 657-3765. Beamtime proposals can be submitted at ***www.lightsource.ca/uso/.***

Huber psi-8 diffractometer, under commissioning.

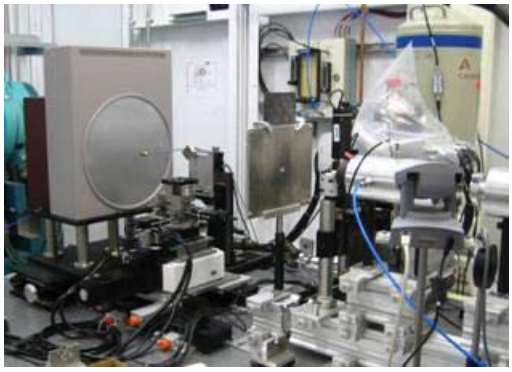
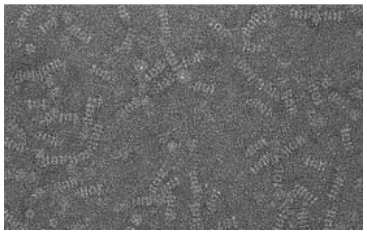


Image plate detector.

The Canadian Centre for Electron Microscopy provides world-class electron microscopy capabilities and expertise to Canadian and foreign researchers working on a broad range of materials research.

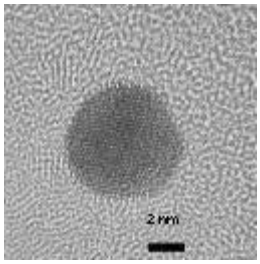
One of CCEM's two ultrahigh-resolution electron microscopes, built in The Netherlands by the company FEI. Equipped with an aberration corrector, this instrument was delivered in June 2007 and achieved 0.75Å information limit resolution within 5 days of being delivered to McMaster.

Instrumentation: FEI Titan 80-300HB TEM, FEI Titan 80-300 TEM (both systems can operate sample holders from near-liquid He temperature up to 1000^{0}C and imaging plates for low-dose imaging), JEOL 2010F TEM, VG HB601 UHV STEM, Philips CM12 conventional TEM

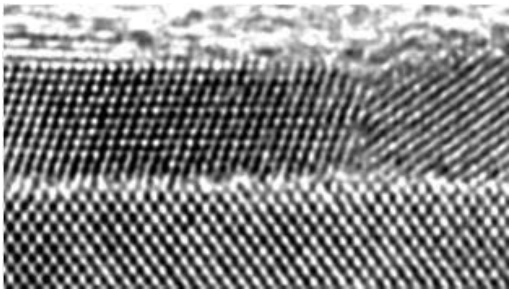


Cryomicroscopy micrograph of ClpXAP protease complexes from Escherichia Coli (courtesy of J. Ortega, CCEM).

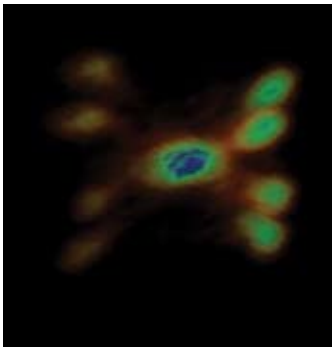
The Centre also provides access to scanning electron microscopes equipped with EDS, EBSD and electron beam lithography, scanning probe microscopes, confocal and light microscopes with image analysis capabilities, and a range of sample preparation equipment. Knowledgeable staff provide training and expert advice on the operation of these instruments. CCEM's computer cluster is dedicated to image interpretation and simulation as well as calculation of energy loss spectra, EDS and EBSD analysis.



Nanoparticle of AuAg produced by laser ablation in a liquid.



Interface between an oxide and semiconductor for the next-generation transistors.



Phase change of Ni-Mn-Ga film (004 reflection) from cubic to twinned tetragonal.

Collaborations The projects of CCEM are collaborative efforts currently underway among universities and research centres within Ontario, across Canada, and internationally. The CCEM brings international researchers to McMaster University, leading to productive interactions with other users of the facility. As an additional benefit, collaborations make it possible for Canadian users to access other international facilities and be part of a global network of super-microscopes not available to one single country.

More than 100 researchers from 24 universities across Canada and 12 national laboratories use this state-of-the-art facility.

The combination of electron imaging and microdiffraction with x-ray diffraction and texture analyses allows for rapid characterization of thin films.

CCEM Funding Partners: Canada Foundation for Innovation; Ontario Government (Ministries of Research and Innovation; Economic Development and Trade; Ontario Innovation Trust); McMaster University.

For further information contact: ***Gianluigi Botton - gbotton@mcmaster.ca - (url) brockhouse.mcmaster.ca.***

Reminder*:** We are planning to hold 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***).

Jim Britten

James Cline receives the 2008 ICDD Fellow Award: ***James Cline*** (National Institute of Standards and Technology (NIST) was named as an ICDD Fellow at the spring meeting in Newtown Square, PA. The increased quality of powder data in the ICDD database is directly associated with the use of Standard Reference Materials (SRMs) developed and certified by Jim Cline. In the 20 years Jim has led the NIST X-ray Metrology Standards Program several well established NIST SRMs have been renewed, and several new SRMs have been certified with improved artifacts and reduced error bounds on certified parameters. These improvements have enhanced the accuracy and precision of diffraction data worldwide. In recent years, the NIST X-ray Metrology Standards Program has grown considerably and, with the certification of SRM 2000, a High-Resolution Diffraction standard, has begun bringing SI traceability to thin films.

Ludo Frevel Crystallography Scholarships: To encourage promising graduate students to pursue crystallography oriented research, the ICDD has established the Ludo Frevel Crystallography Scholarship Fund. Multiple recipients are selected on a competitive basis, each receiving an award of $2,500.

One of the the 2008 scholarship recipients is ACA member ***Katherine Snoda Ryan*** (Massachusetts Institute of Technology). This is Kaity's second year as a scholarship recipient; she was also a 2007 awardees. Her research centers on using macromolecular crystallography to investigate enzymes that biosynthesize a class of anti-tumor natural products called indolocarbazoles. "Using structural data, I study the mechanisms by which these enzymes interact with unstable substrate molecules, acting to both prevent spontaneous, unwanted chemistry and to promote the production of desired compounds. This work should help us to understand how nature builds these molecules, which might lead to new synthetic strategies or to studies in protein engineering."

Magdalena Korczynska (McGill University, Montreal, Canada) was also selected as a 2008 scholarship recipient. Her reserach involves the structural characterization of potential drug targets." Magdalena also received a travel grant to attend the ACA meeting in Salt Lake City where she was selected as one of the poster prize recipients.

ICDD Board: L to R Front Row: Director-at-Large - Evgeny Antipov (Moscow State University), Director-at-Large - Paolo Scardi (University di Trento), Treasurer – David Taylor, Chairman - Thomas Blanton (Eastman Kodak), Past Chairman - James Kaduk (INEOS Technologies), Executive Director -Timothy Fawcett (ICDD), Director-at-Large - Davor Balzar (University of Denver), Director-at-Large - Mark Rodriguez (Sandia Natl. Labs), Corporate Secretary - Theresa Maguire (ICDD). L to R Back Row:Director-at-Large - John Faber, Vice Chairman - Raymond Goehner (Sandia Natl Labs), Chairman, Technical Committee - Scott Misture (Alfred Unviversity).

Travel Grants Available

The International Structural Genomics Organization (ISGO, ***www.isgo.org***) is pleased to announce that ten ISGO - NIH Protein Structure Initiative Student Travel Fellowships are available for travel to the ICSG 2008 conference in Oxford, UK, Sept 20-24, 2008 (***www.spine2.eu/SPINE2/ISGO/***).

Young scientist travel support of up to $1000 US will be made available to graduate students and young post-doctoral researchers to attend ICSG 2008. A total of 10 ISGO - NIH Protein Structure Initiative Student Travel Fellowships have kindly been provided by the ISGO and the NIH Protein Structure Initiative. Applications for young scientist travel fellowships should be made by supplying the following documents:

An abstract and a brief CV.

A cover letter explaining why the applicant should be considered for a fellowship.

A supporting letter from the applicant's academic supervisor, including confirmation of student or post-doctoral status.

The deadline for application is ***July 15th, 2008***, and applications should be emailed to Tom Terwilliger ***(terwilliger@lanl.gov).***

Please note: applications for young scientist travel fellowships will be evaluated by committee and awarded to those judged to be the most deserving candidates. Applications submitted without the accompanying documents will not be considered. Fellowships will be announced by Aug 15, 2006., and provided as travel reimbursements ***after the meeting***. Successful applicants are still required to register in the usual way and are responsible for their own registration, accommodation and travel expenses.

A Thank You from Uruguay

We would like to make public our thanks to ***Mark Sanderson*** (Randall Division of Cell and Molecular Biophysics, King's College London) for his kindness and the donation of a Rigaku DXG2 Generator to our group at the Crystallography, Solid State and Materials Laboratory (*Cryssmat-Lab*), School of Chemistry, Universidad de la República, Montevideo, Uruguay. This would not have been possible without the *ACA Reflexions* magazine, that published the announcement on page 10 of the Fall 2007 issue. This generator will allow us to replace an old Nonius Diffractis 582 generator that had been donated to our lab. in 1991 and is still being used to feed X-rays to a Rigaku AFC-7S four circle diffractometer used for small molecule single crystal x-ray diffraction. This generator will be a significant contribution to our current work and the formation of the next generation of chemical crystallographers in Uruguay. Many thanks.

We would also like to use this opportunity to explore the interest in donating or selling us (second hand) a chiller able to feed cooling water to the Rigaku DXG2 Generator mentioned above. We would pay for shipping from donor's/seller's location. Please, email ***amombru@fq.edu.uy*** or ***leopoldo@fq.edu.uy*** if interested. Thanks again in advance to *ACAReflexions*.

Leopoldo Suescun & Alvaro W. Mombrú

Writing in the Boston Globe (May 8, 2008), Kenneth R. Miller blasts the creationist propaganda film Expelled, writing, "American science is in trouble, and if you wonder why, just go to the movies. Popular culture is gradually turning against science, and Ben Stein's new movie, '*Expelled*,' is helping to push it along." "There are many things wrong with this movie," Miller observes, citing not only its errors of fact but also its deliberate misrepresentation of science as atheistic: "showing a scientist who accepts both God and evolution would have confused their story line."

Moreover, Miller continues, "by far the film's most outlandish misrepresentation is its linkage of Darwin with the Holocaust. A concentration camp tour guide tells Stein that the Nazis were practicing 'Darwinism,' and that's that. Never mind those belt buckles proclaiming Gott mit uns (God is with us), the toxic anti-Semitism of Martin Luther, the ghettoes and murderous pogroms in Christian Europe centuries before Darwin's birth."

After quoting Expelled's spokesman Ben Stein's bizarre claim that "Science leads you to killing people," Miller concludes, "'*Expelled*' is a shoddy piece of propaganda that props up the failures of Intelligent Design by playing the victim card. It deceives its audiences, slanders the scientific community, and contributes mightily to a climate of hostility to science itself.

Miller, a professor of biology at Brown University, coauthored the most widely used high school biology textbooks in the United States. He is also the author of *Finding Darwin's God* and the forthcoming *Only a Theory: Evolution and the Battle for America's Soul*.

International News

Turkey: Adnan Oktar, the Islamic creationist who writes under the pseudonym "Harun Yahya," was sentenced by a Turkish court to three years in prison for "creating an illegal organization for personal gain," according to a report from Reuters (May 9, 2008). The charges reportedly stemmed from a previous trial in which Oktar was "charged with using threats for personal benefit and creating an organization with the intent to commit a crime." A spokesperson for BAV confirmed the fact of Oktar's sentencing to Reuters, but claimed that the judge was influenced by pressure groups and stated that Oktar would appeal the verdict.

England: In a statement issued on April 11, 2008, the Geological Society of London denounced young-earth creationism, "creation science," and "intelligent design" as "a trespass upon the domain of science," and described the scientific estimates of the age of the earth and when life forms first evolved. In addition, close study of the structure and organization of living animals and plants clearly indicates their common ancestry, and the succession of forms through the fossil record, as well as the genetic record contained in every living organism, provides powerful evidence of the reality of evolution."

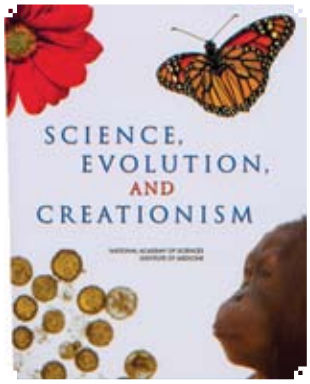
In the US

May 2008: Antievolution bills died In Florida

Aprril 2008: Creationist lawsuit against Woods Hole dismissed; antievolution legislation proposed in Michigan and Alabama; Louisiana antievolution bill passes Senate; ICR fails to obtain certification in Texas; a new antievolution bill in Missouri; interim victory in California creationism case.

Publications

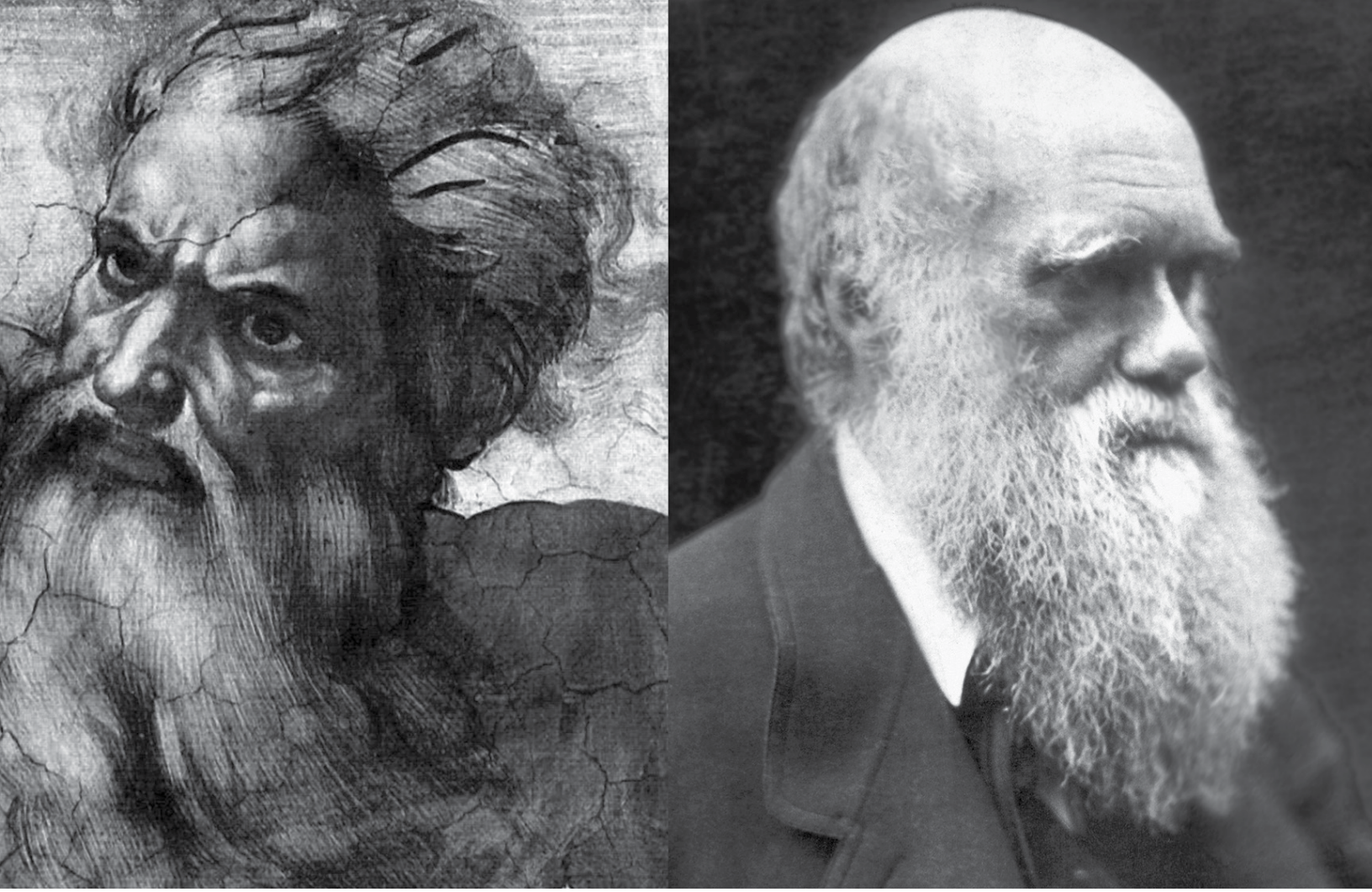
The second issue of *Evolution: Education and Outreach* -- the new journal aspiring to promote accurate understanding and comprehensive teaching of evolutionary theory for a wide audience -- is now available on-line (***www.springerlink.com/content/120878/***). Featured are original scientific articles on such topics as evolutionary medicine, evolutionary trees, and punctuated equilibrium; curriculum articles on such topics as using *Inherit the Wind* in the science classroom, molecular evolution and HIV, and hominid evolution; and reviews of a host of books, including David Sloan Wilson's *Evolution for Everyone* and Philip Kitcher's *Living with Darwin*. Those interested in the intersection of science and art will enjoy a report on Esther Solondz's *The Evolution of Darwin* installation (***www.bu.edu/darwin***) as well as a description of a project fusing evolutionary biology with ceramics and printmaking.



The National Academy of Sciences and the Institute of Medicine haved jointly released *Science, Evolution, and Creationism*. The book provides a comprehensive and up-to-date picture of the current scientific understanding of evolution and its importance in the science classroom. It includes the many fascinating inquiries being pursued that put the science of evolution to work in preventing and treating human disease, developing new agricultural products, and fostering industrial innovations. It also presents the scientific and legal reasons for not teaching creationist ideas in public school science classes. Mindful of school board battles and recent court decisions, *Science, Evolution, and Creationism* carefully explains why science and religion should be viewed as different ways of understanding the world rather than as frameworks that are in conflict with each other and that the evidence for evolution can be fully compatible with religious faith. ISBN-13: 978-0-309-10586-6; ISBN-10: 0-309-10586-2: *x10, 88 pages. Paperback version: $12.95 (with multiple copy discounts available); PDF version: free at ***www.nap.edu/sec***. Summary version: An 8-page brochure is available free and in print and as a PDF from the same website. More information on NAS activities in the area is available at ***nationalacademies.org/evolution***).

Acknowledgement

The NCSE (National Center for Science Education) website (***www.natcenscied.org/***) for the leads to the review of *Expelled,* details on national and international legal proceedings and the link to *Evolution: Education and Outreach.*



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Protein Crystallography: A Concise Guide (2008) E. Lattman and P. Loll, Johns Hopkins Univ. Press (ISBN: 0801888069)

"Why another book on protein crystallography?" This is a good question and is the opening line of *Protein Crystallography, A Concise Guide*, by Eaton Lattman and Patrick Loll. The authors' rationale for writing the book is a belief in the "demand for a concise, accessible introduction to this powerful method". They have accomplished this with an elegance derived from simplicity. In some 130 pages, the reader is taken from a physical understanding of x-ray diffraction via phasing through to the refinement of the resulting model. The first chapter introduces crystallography as an imaging technique, which is followed by a chapter on the physical basis for understanding diffraction and then a chapter bringing three dimensions into play. These provide the groundwork for the remaining four chapters covering isomorphous replacement, the Patterson function, the use of partially known structures and the process of structural refinement. These chapters are not intended as comprehensive practical guides; instead, they provide the basis and depth for understanding the general methodology and calculations involved. This is essential to grasp the practical aspects completely. The text is clear and concise, and covers the theory and the language used in the field. Importantly, it does not shy away from mathematical detail where that detail helps the explanation. Each chapter is well illustrated with clear figures. At the end of each chapter, there is a summary of the important facts and an up to date list of further reading. The lists are annotated with a brief description of the focus of the text and the occasional comment on arctic adventures or the values of old textbooks!

One notable feature is the extensive glossary, which gives a very detailed explanation of the terms routinely used in crystallography. This provides a useful guide to the language used in the field, especially for those who could benefit from, but are not familiar with the techniques. The book is very suitable course material for an introduction to crystallography at an advanced undergraduate level or as the basis of a more expansive course at the graduate level. It is gratifying to see such a nice piece of work and the book is highly recommended.

Eddie Snell

Powder Diffraaction Theory and Practice (2008) R. E. Dinnebier and S. J. L. Billinge, Eds., RSC Publishing (ISBN:9780854042319)

For most of the past century, powder diffraction was a lesser branch of crystallography, a powerful technique for problems such as phase identification and quantification, but used only infrequently for structure determination or quantitative determination of microstructural properties such as texture, strain, and stress. Continuous developments, such as parafocusing x-ray diffractometers, the Rietveld method, parallel beam x-ray optics, spallation neutron sources, and a wealth of computer software, have vastly strengthened powder diffraction in its traditional domain, as well as allowing it to develop into a method of structure determination nearly as mature and powerful as single crystal techniques. That development has been documented and guided by a number of excellent books on the technique; it is a pleasure to welcome and recommend the newest of these, *Powder Diffraction Theory and Practice*, edited by Robert Dinnebier and Simon Billinge.

This book complements the excellent tutorial *Fundamentals of Powder Diffraction and Structural Characterization of Materials* recently published by Pecharsky and Zavalij. It is probably not the place to start to learn about the principles of powder diffraction, but as a researcher embarks on independent work in the field, the chapters are an excellent place to learn current practice, which is often difficult from the primary literature. Something like half of the book is on topics overlapping the coverage of *Structure Determination by Powder Diffraction*, edited by W.I.F. David et al., but many aspects of structure determination have evolved significantly since that book's 2002 publication. The other half, including descriptions of quantitative phase analysis, microstructural properties, and total scattering, are very welcome here. The organization is also excellent, for example with separate chapters on data reduction in general, line profiles for intensity extraction, microstructural information from line profiles, and instrumental contributions to diffraction line profiles.

Considering one topic covered, familiar methods of quantitative phase analysis are based either on the Rietveld method (crystal structures of all phases known, no need to measure standards on the same instrument) or the reference intensity ratio method (standard pattern measured under similar experimental conditions). However, if one of the analyte phases is of unknown structure and/or poorly crystalline relative to standards that have been examined this is a more complicated problem that would probably come as a rude shock to many practitioners. The chapter on quantitative phase analysis by Madsen and Scarlett addresses this issue in a way that provides real guidance to somebody facing such a problem. It also gives an excellent overview of the accuracy and precision of results from x-ray quantitative phase analysis.

Cranswick's chapter on computer software is an outstandingly valuable contribution to the community. A major part of the growth of the powder diffraction technique has come from developments in software, and he provides a critical review with useful advice for anybody - rookie or veteran. Alas, the field is probably advancing sufficiently rapidly that it will become dated before long, but it will remain useful to people wanting to sample what is available.

The authors of chapters have done a very good job of summarizing current ideas in the field of powder diffraction, and the editors and publisher have likewise maintained the coherence, consistency, and quality of the finished product. *Powder Diffraction, Theory and Practice* provides an excellent bridge between elementary texts and current research literature. I believe that there is room for this book on the shelf (and more importantly, in the hands) of nearly everybody who is using powder diffraction as a research technique.

Peter W. Stephens

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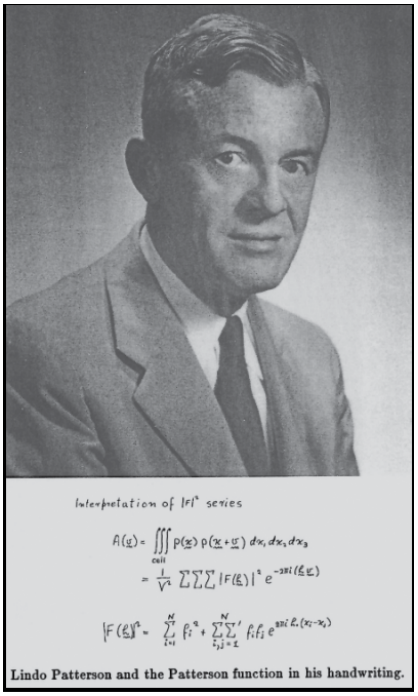
think forward

Crystallography

A. L. Patterson



Lindo Patterson and the Patterson function in his handwriting.

Lindo Patterson, in articles published in 1934, showed how it was possible to determine interatomic distances in a crystal by use of a Fourier calculation involving values of $|F|^2$ (which are phaseless) as coefficients. Thus, structural information can be obtained without any knowledge of the relative phases of the diffracted beams. It was immediately recognized that a method had, at last, been proposed that could be used to solve larger structures, and the method was eventually to play an important role in the subsequent determinations of protein and virus structures. The technique for structure solution had been changed from a trial-and-error procedure to an analytical procedure.

There is a story that J. M. Robertson and Lindo shared a room during the April 1950 conference at State College on "Computing Methods and the Phase Problem" run by Ray Pepinsky. Lindo drove there late one evening when Robertson had already retired and locked the door. When Lindo knocked on the door and woke him, Robertson said: "I see before me a dimly resolved Patterson." There is space here for only a few aspects of his life, giving only a "dimly resolved" view of this great man.

Historically, the first big step toward crystal structure determination came when von Laue, as a result of Barkla's work on x-ray polarization, estimates of x-ray wavelengths and his own earlier work on scattering from periodic structures, realized that if x-rays were wavelike rather than particle-like, they could be diffracted by crystals. This was demonstrated by Friedrich and Knipping. The second step was taken by W. L. Bragg when he realized that the internal structure of the crystal could be determined from the x-ray diffraction pattern. Interatomic distances could also be measured if the x-ray length is known. Young Bragg asked some chemists which were the interesting structures to do and was sent to see Pope and Barlow. They told him to look at the alkali halides and see if the ions were arranged as packed spheres as they had predicted. As a result the Braggs (father and son) determined the structures of sodium and potassium chloride. Other structure determinations followed in their footsteps and some interesting salts, alloys and organic compounds were studied.

But the crystals had to have simple structures if they were to be determined. The frustrations of the time were very clear. Structures could only be solved if the symmetry of the crystal meant that only one or two general parameters were needed to define the entire structure. For example, Pauling said that when he got to Pasadena in 1922 Dickinson told him that the thing to do in order to get answers to questions was to determine crystal structures. But he also told him that it was easier to determine the structure of a cubic crystal than of a crystal of low symmetry. So Linus crystallized about a dozen cubic crystals in the first few months there. One (cesium mercuric bromide) had 32 molecules in the unit cell in general positions, another (potassium nickel sulfate) had 19 atoms in the asymmetric unit, and a third (the alloy, sodium dicadmium) had 1200 atoms in the unit cell. The next (dimagnesium stannide) had the fluorite structure so that all atomic positions were immediately known. Linus then got tired of not being able to solve the structures of crystals because there were too many parameters that needed to be evaluated and so he, like many others, determined structures by "trial-and-error" methods. A structure was derived by model building or other means, and the agreement between the observed and calculated diffraction intensities was used to test the validity of the proposed structure.

But how could crystal structures be determined more directly? The only hope at that time, as Cork realized when he studied the alums, was the use of isomorphous replacement methods. But such small structures are rarely truly isomorphous even if some metal replacement is possible.

The frustration in not being able to solve more complicated structures was well recognized by Patterson, but he was convinced that there was some information in the diffraction pattern that could be better used to analyze the structure. His paper (on the use of the map described by him as the $|F|^2$ map, but known by us as a Patterson map) was an instant success, and was rapidly used by many for years until direct methods were introduced – but that is another story of other people. The Patterson function is, of course, still used extensively by the macromolecular crystallographers. But even for smaller structures it is often very instructive to study the Patterson map of a compound that cannot readily be solved.

Lindo was born in New Zealand on July 23, 1902 in Nelson (near Auckland) but his family left for Canada when he was eighteen months old. He went to school in Montreal, but when he was 14 he was sent to an English school (public to the English, private to Americans), Tonbridge (1916-1920). He had an older brother who died in World War I of gangrene from his wounds but Lindo was never old enough during the war to serve in the armed forces. However, later, he always hated peanut butter, a reminder of the poor diet at that time.

From Tonbridge he then went to McGill University (1920-1924) where he majored in physics, receiving a bachelor's degree in 1923 and a master's thesis was the production of hard x-rays by the interaction of radium β-rays with solids. He said that his professors decided that the bachelor's degree was not as good as it might be because he had too many friends in Montreal and was addicted to activities such as skiing, bridge, and dancing.

His graduate studies were done under the supervision of A. S. Eve, on "The application of x-rays to the study of organic substances". In 1924 McGill announced the endowment of two Moyse Traveling Fellowships, and one was awarded to Lindo. Lindo's parents were in England, and so he wrote to W. H. Bragg and was able to work with him at the Royal Inst. (R. I.) in London for two years. Bragg was interested in naphthalene and anthracene, and Muller and Shearer were studying long chain compounds. Patterson worked on determination of the unit cell dimensions and space groups (at that time no structure determinations were contemplated) of various phenylaliphatic acids, since these had characteristics of both sets of compounds being studied at the R.I. To do this he had to build his own x-ray equipment.

The Pulp and Paper Industry Research Laboratory at McGill University was interested in the work of Herzog and Jancke on the x-ray diffraction of cellulose and provided Lindo a fellowship for such studies. Therefore he spent a year with Hermann Mark at the Kaiser-Wilhelm Institute in Berlin, on the "particle size" of cellulose. Here he worked on the theory of particle-size line broadening and his contributions were substantial, as shown by a note in *Zeitschrift fur Physik*.

While he was in Berlin in 1926-1927 he kept a diary which shows that music was his first love, but he was very stimulated by the atmosphere provided by all the scientists there and was rapidly able to contribute. At first he had to struggle with the problems of learning German. He wrote "Tonight my landladies have given me some light reading "Fürst Bismarck's Briefe an seine Braut und Gattin" (FTimes Fürst Bismarck's Letters to his Bride and Wife). I really cannot face it so I think that bed is indicated." But later he was able to write "I am very proud to say that yesterday I separated my first prefix successfully. I think that the sensation must be similar to that of a doctor removing his first appendix." His love of music resulted in a very interesting analogy. Lindo wrote: "This leads me rather to a discussion which I had with Mark, and a comparison, I think due to him in the discussion, between music and crystallography. He is not so particularly keen on Bach, from the music point of view and although he acknowledges him as the founder of modern music, only from the mechanical point of view. The comparison is between the mathematical theory of crystallography as developed by Schonflies and von Fedorov, and Bach. The mathematical theory of music was provided by Bach, and just as Fedorov and Schonflies would not have been able to make the beautiful applications of their theories to the interpretations of crystal structure, so was Bach unable to write the *Ninth Symphony*. The *Goldberg Variations* fall very nicely into the analogy, as being space groups of a certain symmetry class. The *Well Tempered Clavichord* is more or less the set of examples appended to show what can be done with the beautiful new mathematics. The *St. Matthew Passion*, and the *Mass*, and the *Bradenburg Concertos* are more difficult to fit in. The two, three, and four piano concertos, are more or less the examples of the cubic system in extension of W.T.C. [*Well Tempered Clavicord*]. Carrying the analogy further, von Laue, Friedrich and Knipping compare with Mozart and Haydn, who found out what could be done with the mathematics in applying it to the expression of these ideas. W. H. and W. L. Bragg acquire the cloak of Beethoven. W. L. [Bragg]'s *Cam. Phil. Soc.* paper and the structure determinations of salt and diamond compare with the first two symphonies of Beethoven, the first, which also might have been written by Mozart, and the second showing the hand of the master. The *Eroica*, when the artistic sense of the master begins to take hold, one can compare with the application of the work to the organic substances. Fedorov, Schonflies or even Laue would have wanted a little more to go on, but the application of the touch of the artist brought about this beautiful work, which may lack the preciseness of geometrical definiteness, but which is truth for all that. The work of W. L. Bragg on beryl, I should say, ranks very high in the string quartets of Beethoven when we carry the comparison on, but I am afraid, that the V and IX Symphonies have yet to be written." Remember that Lindo wrote this in Germany, long before the Patterson function was thought of!

Lindo enjoyed the scientific atmosphere in the Germany of the times (1926-1927) and wrote: "There really are an amazing collection of "wissenchaftliche" stars here in Dahlem. At the colloquium in Haber Institute there were: Haber, Freundlich, Weissenberg, Polanyi, Hahn, Meitner, and then they were not nearly all met as the session has not really got going. The Berlin Physics Colloquium is I believe absolutely magnificent. One name only need be mentioned, and that is Einstein, but there are many others. Today I assisted in the setting up of a new tube, and find that troubles are more or less the same the world over. Today I think for the first time I succeeded in cracking a joke in German without having to explain it about three times; I also succeeded in making a successful pun, so I am feeling pretty good." His further description of the scientific atmosphere is described as follows: "In the afternoon, I went to my first Phys-

ics Colloquium in the University. Einstein, Laue, Planck, Nerst, form the nucleus, with goodness knows how many other stars. It really was wonderful. I understood most of everybody but Laue, and the Germans themselves find him difficult to follow. Einstein is quite a cheery soul. I met Ewald who is a first rate sort, who speaks, as do most people, about 3 languages fluently. I don't think that even in the R.I. or at the B.A. I have ever been in the same room with so many scientific bloods. They all seem quite ordinary people, but Einstein and he seems extremely human in character, but he has one of the most marvelous faces of anyone I have ever seen. A perfectly marvelous head as well. There is a photograph of him in a shop in the Uhlandstrasse that I would like to buy, but I don't know if such is allowed. When you see the man you realize how it is possible that he has done such wonderful work."

On Good Friday in 1927 the Davisson and Germer paper on the diffraction of electrons was read by Lindo. He describes he events as follows: "Sat 16th received copy of *Nature* with Davisson's paper and made everybody's life miserable with my enthusiasm. Sunday, went to Potsdam with Stark [whom he describes as S] and talked Davisson. Monday we worked Davisson's paper out completely. Nothing of note seems to have happened then until Friday 29th Apr. When someone rang me up, (later found to be S). Saturday W came and asked me for my copy of *Nature* with the Davisson paper in it (for S). Monday at the Wellenmechanik Colloq. I gave it up to him. Wednesday before the Colloquium I asked S if Laue was going to speak on the Davisson paper. He said no. I had invited the Rosses to the Colloquium to look at the Lions. As soon as the Colloquium started Laue started off very dramatically with the Davisson work. Announced that they had obtained interferences from single crystals with electrons. Sensation! Much discussion, in which someone asked Laue if anything was said about velocities, he said no, I put up my hand and said yes. Laue goes on with the discussion of the paper and gets it all wrong, bad English and general unclearness in the paper being the cause. He said they had used the wrong lattice constants, that the effect did not agree with a surface reflection. I tried to speak, but everyone was talking at once, and I did not get a chance to speak until Pringsheim, called Laue's attention to the fact that I wanted to speak. He then called on me, and I got up and told him that I had worked the thing through and it all agreed perfectly. He said that he and S had worked it out and it didn't agree. I am inclined to think that S lead him astray. It was lucky that I knew the paper by heart, as S had my copy the whole time. After my remarks, Laue said that as I read the paper so thoroughly I had better come and talk about it. Which I did, with the worst wind up which I have had for a long time. I talked for about 15 minutes."

He was so scared, Lindo related later, when he talked about the Davisson and Germer paper that "the first line he drew on the blackboard came out dotted."

Lindo returned to McGill in 1927 and finished his Ph.D. in 1928. He then was a demonstrator in the physics department for a year. He moved to the Rockefeller Institute in New York and Thomas White, his student from McGill, accompanied him. They worked in R.W.G. Wyckoff's group on cyclohexane derivatives, mainly hexols, from 1929-1931. But he wrote that he had an "obsession with the notion that something was to be learned about structural analysis from Fourier theory." So in 1930 he spent many hours looking through the tables of contents of all the mathematical journals in the New York Public Library, searching for some clues on how he should proceed.

After two years at the Johnson Foundation in Philadelphia studying biological systems he decided he had saved up enough money to be able to work independently on the problem of solving structures and so he went as an unpaid guest scientist to Bert Warren's laboratory at M.I.T. He was particularly interested in going there because he could talk to Norbert Wiener who, he said, "knew as much about Fourier integrals as anyone in the world." His main interest was in the Faltung or convolution and its Fourier transform. He discussed Fourier integrals with Wiener while singing Gilbert and Sullivan operas. In fact he put the words of the question he had into the music of the song they were singing together. Lindo asked Norbert Wiener "What do you know about a function representable by a Fourier series when you know only the *amplitudes* of the Fourier coefficients?" Wiener's laconic reply was "You know the Faltung."

Lindo wrote "The understanding of the Faltung came, of course, from the work on liquids and their radial distributions. Warren with Gingrich and others had perfected the techniques used by Debye and Menke in the study of the x-ray scattering from liquids. These were of course based on the original suggestions of Zernike and Prins. Warren and Gingrich had already had the idea that these methods applied to powders would give the radial distribution in a crystal. While trying to learn about their work I noticed that the mathematical form of the theory given by Debye and Menke would be identical with that of the Faltung if the integrations over random orientation were left out and the randomness of choice of origin was left in. What was immediately apparent was that the crystal contained atoms and that the Faltung of a set of atoms was very special in that it would consist of a set of atom-like peaks whose centers were specified by the distances between the atoms in the crystal." Thus the Patterson or $|F|^2$ series was proposed.

He continued, "All this happened on a Tuesday, and Friday was the deadline date for the Washington spring meeting (1934) of the American Physical Soc.. An abstract had to be prepared in a hurry to go in with that of Warren on the radial distribution in carbon black and that of Gingrich and Warren on the radial distribution in powders which was basic to my work. The only $|F(h)|^2$ – series which I was able to compute [with the primi-

tive computing equipment of the time] in the month between the deadline and the meeting was the (hk0) of KH_2PO_4 and a one-dimensional series for a simple layer structure. All three papers were very well received and had full discussion with A.H. Compton in the chair and W.L.Bragg in the audience to ask the right questions."

It was tedious and time-consuming to compute such Fourier maps and therefore Patterson, with George Tunell, devised the Patterson-Tunell strips, similar to the Beevers-Lipson strips of the English crystallographers. Then it was possible to compute Patterson maps (generally only in projection) for a whole series

of compounds. However, Lindo was always sorry that he had not thought of the fact, noticed by Harker, that certain areas of the Patterson map contain a lot of structural information.

Due to the depression, Lindo had been 3 years without a job, until he joined the faculty of the physics dept. at Bryn Mawr College, near Philadelphia. His colleague was Michels, who was interested in solid state physics. The combination of names meant that they were affectionately called "Pat and Mike." Together they wrote a textbook. In this textbook there are some out-of-the-ordinary diagrams, including a schmoo (drawn by Al Capp), to illustrate Gauss' law and a Charles Addams child (with no neck) illustrating the principle of the solitary see-saw. The year before going to Bryn Mawr, Lindo married Betty Knight, whom he had met at the Rockefeller Institute. She was a lively and active scientist interested in the biochemistry of enzyme reactions.

During the war, the government was interested in the mining of harbors and the effects of waves on the triggering of these explosive devices. Lindo worked on thiswith Michels, who was a Commander in the Navy, first at Bryn Mawr, and later in Washington (as a foreign national) for the U.S. Naval Ordinance Bureau. In 1945 he received the Meritorious Civilian Service Award for his work on submarine warfare. He became a U.S. citizen in the same year.

After the war he continued his main interests which were particle-size line broadening and the study of "homometric structures." These are different atomic arrangements with the same Patterson function. Pauling tells the story of this. Apparently about the time that the Patterson function was first published Linus had a graduate student who was studying bixbyite, originally studied by Zachariasen. This structure contains 32 metal atoms and 48 oxygen atoms in the unit cell. Linus discovered that in bixbyite the metal atoms could be arranged in two physically quite distinct arrangements that gave exactly the same calculated x-ray diffraction pattern. So, when he read, in a copy of *American Physical Society Bulletin*, about a meeting, he found that Lindo planned to present a proof that no two physically distinct structures can have the same Patterson map or diffraction pattern. So he wrote to Lindo saying that he had an example of two structures that were physically distinct but that had exactly the same Patterson diagram, and when Lindo gave the paper the following month it was on the conditions under which two structures can have the same Patterson map.

In 1949 he came to the Inst. for Cancer Res. where he studied t compounds of biological interest, such as citrates. But his interest in homometric structures continued, and he was working on the development of a theory on them when he died.

Lindo served the ACA with great dedication throughout its history and played an important role in its formation in 1950 when the American Society for X-ray and Electron Diffraction (ASXRED) and the Crystallographic Society of America (CSA) merged. He was President of ASXRED in 1949 and served on the ACA Publications Committee in 1955-1957 and 1959-1961. Another great service to the Crystallographic Community was his section on "Fundamental Mathematics" in Volume II of "*International Tables*." He contributed to international crystallography by his service on the USNCCr in 1951-1955, 1957-1962, and 1964-1966. He was a major writer of the by-laws of the IUCr.

Lindo died suddenly and unexpectedly of a cerebral hemorrhage in November 1966 at the age of 64. Unfortunately, although he was very goodlooking, not many good photographs of him remain. He tended to "freeze" in front of a camera and his dynamic character was lost in the resulting photograph.

Of course, the insight gained from his scientific discoveries tells us nothing of the kind of person he was. How would he appear to each of you at a meeting? He was a tall, thin, freckled, redhead with a ready smile, and yet he could be firm. Even though crystallographers are particularly nice and friendly people, he ranked among the best for friendliness, thoughtfulness and integrity. He almost never had a bad word to say about anyone, and no one said a bad word about him. The older members of ACA knew Lindo well because he was an active member, attended all meetings, and made sure he had a word of encouragement for new young crystallographers giving their first papers. He also gave young scientists an opportunity to meet older scientists and to take part in discussions at a level that might otherwise not have been possible to them for many years. Yet he was shy and was always nervous in a meeting before he asked a question.

He thoroughly enjoyed good conversation, good food, and good music. He could sing most of the Gilbert and Sullivan arias, having acted in productions of these operettas in his earlier years. He had a delightful sense of humor and said that the best crystallographic information was obtained by informal discussion, preferably at the bar. That was in the days before poster sessions.

At one stage he became tired of reading lots of acronyms and yet realized that jargon was taking over crystallography and therefore wrote an article, signed A.L. Pon, in which he tried to save space by condensing words. The article, which is very readable, was accepted by *Acta* since it was good science, but, since there were financial problems in publishing *Acta* at that time people had been requested to shorten papers. As a result, he withdrew it, but offprints marked "Not reprinted from *Acta Crystallographica"* were produced. A "translation" is in order.

"On the symmetry of white radiation streaks produced by the Buerger precession camera" by A. L. Patterson, Senior Member, Department of Physics, Institute for Cancer Research, Philadelphia, Pennsylvania, U. S. A.

> Recent publications on the reciprocal lattice theory of diffracted reflections of x-rays have suggested the mathematical techniques used in the preliminary note.
>
> It is clear that in all discussions of diffraction problems, the radius of the Ewald sphere can be set at unity (Verner Schomaker, unpublished). If then a given reciprocal lattice point is associated with monochromatic radiation of a given wavelength, then a reciprocal vector, joining this reciprocal lattice point with the reciprocal lattice origin corresponds to the white radiation which is necessarily produced with the monochromatic radiation in the x-ray tube (see any textbook on quantum theory). Thus any diffraction phenomena produced by the Buerger precession camera possesses plane symmetry about a symmetry plane through the reciprocal lattice point, the reciprocal lattice origin and the diffracted ray" (Not reprinted from *Acta Crystallographica*).

Jenny P. Glusker

RefleXions Inside and Out

The ACA Patterson Award was presented to B.C. Wang (Georgia Tech) at the ACA Meeting in Knoxville. Therefore, as part of our project to publish articles on the history of crystallography it seemed only fitting to include the biography of Patterson in this issue of *RefleXions*. The article, by Jenny Glusker, was originally published in *Crystallography in North America* (1983) D. McLachlan, Jr. and J. P. Glusker, Eds, American Crystallographic Association.. The history of crystallography is also reflected in the cover of the issue of RefleXions which mixes some randomly chosen basic formulas of crystallography with images of the proteins chosen by David Goodsell to highlight the 100th edition of the PDB Molecule of the Month (MOM) series. One has to wonder what Bragg, Ewald and Patterson and the other early crystallographic pioneers would think about the wwPDB archive of protein structures containing more than 50000 entries (see page 33) and the CCDC fast approaching 500,000 small molecule structures. References for the structures in the MOM article (see page 34) are: Fig.1 – **2RH1** -Cherezov, V., Rosenbaum, D.M., Hanson, M.A., Rasmussen, S.G., Thian, F.S., Kobilka, T.S., Choi, H.J., Kuhn, P., Weis, W.I., Kobilka, B.K., Stevens, R.C. (2007) High-resolution crystal structure of an engineered human beta2-adrenergic G protein-coupled receptor. *Science* **318**: 1258-1265; Fig.2 – **1FFK** -Ban, N., Nissen, P., Hansen, J., Moore, P.B., Steitz, T.A. (2000) The complete atomic structure of the large ribosomal subunit at 2.4 A resolution. *Science* **289**: 905-920 and **1FKA** - Schluenzen, F., Tocilj, A., Zarivach, R., Harms, J., Gluehmann, M., Janell, D., Bashan, A., Bartels, H., Agmon, I., Franceschi, F., Yonath, A. (2000) Structure of functionally activated small ribosomal subunit at 3.3 angstroms resolution. *Cell* **102**: 615-623; Fig. 3 – **1MBN** - Watson, H.C. (1969) The Stereochemistry of the Protein Myoglobin *Prog. Stereochem.* **4**: 299; Fig. 4 – **1A3W** -Jurica, M.S., Mesecar, A., Heath, P.J., Shi, W., Nowak, T., Stoddard, B.L. (1998) The allosteric regulation of pyruvate kinase by fructose-1,6-bisphosphate. *Structure* **6**: 195-210; and Fig. 5 – **2GBL** - Pattanayek, R., Williams, D.R., Pattanayek, S., Xu, Y., Mori, T., Johnson, C.H., Stewart, P.L., Egli, M. (2006) Analysis of KaiA-KaiC protein interactions in the cyano-bacterial circadian clock using hybrid structural methods. *Embo J.* **25**: 2017-2028

Contributors to this Issue

Paul Anderson, Alicia Beatty, Jim Britten, Charlie Carter, James Cline, Louis DelBaere, Jeff Deschamps, Jenny Glusker, David Goodsell, Marv Hackert, Judy Kelly, Cora Lind, Patrick Loll, Alvaro Mombrú, Bill Ojala, Allen Hunter, Thomas Proffen, N.S. Rao, John Rose, David Rose, Eddie Snell, Peter Stephens, Leopoldo Suescun, Tom Terwilliger, Carrie Wilmot, Winnie Wong-Ng, Christine Zardecki

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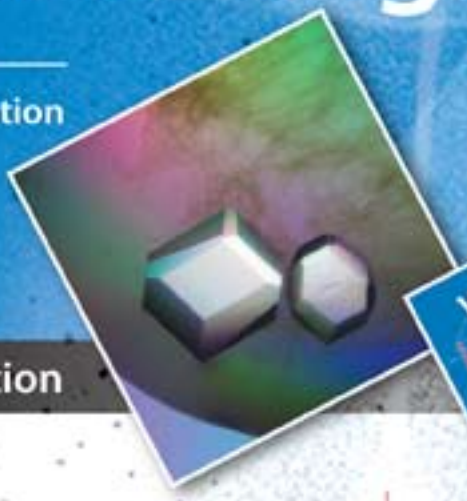

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AMERICAN CRYSTALLOGRAPHIC ASSOCIATION, INC.
BALANCE SHEET - December 31, 2007 and 2006

	CURRENT FUNDS (2007)		TOTAL	
	Unrestricted	Restricted*	All Funds	
			2007	2006
ASSETS				
Current Assets:				
Cash	283,297		283,297	251,432
Investments	326,543	378,753	705,296	679,446
Inventory	5,600		5,600	5,600
Total Current Assets	615,440	378,753	994,193	936,478
Fixed Assets:				
Computers and Printers	4,598		4,598	4,598
Office Equipment	1,300		1,300	1,300
Accumulated Depreciation	0		0	0
Total Fixed Assets	5,898		5,898	5,898
TOTAL ASSETS	621,338	378,753	1,000,091	942,376
Liabilities:				
Deferred Dues Income	82,772		82,772	14,138
Total Liabilities	82,772		82,772	14,138
Fund Balance:				
Unrestricted	538,566		538,566	565,534
Restricted		378,753	378,753	362,704
Total Fund Balance	538,566	378,753	917,310	928,238
TOTAL LIABILITIES & FUND BALANCE	621,338	378,753	1,000,091	942,376

*** Current Balances in individual restricted funds - as of December 31, 2007**

Buerger Award	38,814
Etter Award	66,683
Fankuchen Award	67,578
Patterson Award	43,987
Pauling Award	34,107
Supper Award	11,360
Trueblood Award	33,145
Warren Award	31,273
Wood Science Writing Award	51,606

A more detailed report on the ACA finances may be obtained by sending a written request to the ACA office in Buffalo, PO Box 96, Ellicott Station, Buffalo, NY

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Judy Kelly
Vice-President

Professor Emerita, Department of Molecular and Cell Biology, Member of the Institute for Materials Science, University of Connecticut, Storrs, CT 06269-3125.

Education: AAS (1971) Oakland College (Mathematics/Science); BA (1973) University of Connecticut (Chemistry); PhD (1977) University of Connecticut (Biophysics, with James R. Knox); Postdoc (1977-79) University of Alberta with Michael N. G. James.

Professional Activities: (1979-80) Research Fellow, University of Liege, Liege, Belgium; (1980-2003) Research Associate I to Full Professor, University of Connecticut, Storrs, CT; (1989) Visiting Senior Fellow, University of Oxford, Oxford, England; Fellow, Linacre College, University of Oxford; (1990-92) Acting Department Head – (1992-97) Department Head, Department of Molecular and Cell Biology, University of Connecticut, Storrs, CT; (1995-) Member, The Connecticut Academy of Arts and Sciences; (1996-98) Chair, ACA BioMac SIG; (1997) Fulbright Senior Research Scholar; (1997-1998) Visiting Scientist, Commissariat à l'Energie Atomique, Grenoble, France; (1998) Visiting Professor, University of Copenhagen, Denmark; (2003-)-Professor Emerita, Department of Molecular and Cell Biology and Institute of Materials Science, University of Connecticut, Storrs, CT; (2006) Program Chair, ACA Meeting in Honolulu, HI; (2006-) Volunteer, Maine School Science Volunteers; (2007-) Volunteer, Maine Department of Marine Resources.

Research Interests: The research focus of my career has been on protein structure and function employing the techniques of x-ray diffraction and kinetic methods. Specifically, I have studied enzymes that are targets of antibiotics or are used in the production of drug molecules. My lab has used extensive inhibitor and substrate analog studies to unravel catalytic mechanisms of enzymes. We succeeded in growing protein crystals suitable for ultra-high resolution x-ray crystallographic work. We also have employed neutron diffraction to resolve questions of hydrogen placement in enzyme active sites.

In my volunteer work, I have been involved with Maine School Science Volunteers, a program that places retired scientists and engineers in middle and high school classrooms to assist and to provide expertise to science teachers. In my work with the Maine Department of Marine Resources, I carry out coastal water sampling and analysis to monitor for the toxic algae that are responsible for paralytic shellfish poisoning.

Statement: As I finished high school, the common college majors for women in my peer group were English and History. Knowing I would not be satisfied working in those areas, I chose to go to Berkeley College in New York City and trained to be a secretary. It was a good choice for me at the time. The skills I learned have stayed with me throughout my working life. I landed a great job with The M. W. Kellogg Company, an international engineering company. I worked for the Manager of Government Contract Sales and was involved in interesting projects like the Atomic Energy Commission facility at Idaho Falls. From there, I became the Administrative Assistant to the President of Dover Corporation, a manufacturing conglomerate headquartered in New York City. While working in these positions, I realized I wanted to be involved in the technical side of projects, not the administrative side. So, I began attending college at night school. It took a long time, but it was well worth it because I ended up as a crystallographer – what better world to work in day and night.

As a member of the ACA since the 1970s, I have found participation in our annual meetings to be an important benefit of our organization. Stimulating, informative, and well organized conferences provide the venues for presentation of research results and the essential opportunity to

Candidates for ACA offices in 2009

The Nominating Committee (***Louis Delbaere and Jeanette Krause***) has proposed the following candidates for the 2008 elections for ACA offices in 2009:

Vice-President: **Judy Kelly and Winnie Wong-Ng**

Secretary: **Patrick Loll and Carrie Wilmot**

Committees:

Communicatons: **Alicia Beatty and Thomas Proffen**

Data, Standards & Computing: **Cora Lind and John Rose**

Continuing Education: **Allen Hunter and Bill Ojala**

To nominate write-in candidates for any of these offices, write to the ACA Secretary: Lisa J. Keefe, IMCA-CAT, Sector 17, Bldg. #435A, Advanced Photon Source, Argonne National Laboratory, 9700 South Cass Ave., Argonne, IL 60439. (Fax: (630) 252 0521) Letters must be received by September 15, 2008 and must be signed by 5 supporting ACA members and include a signed statement by the candidate describing his or her qualifications. Statements from all candidates will be included with the ballots which will be sent to all members in October 2008.

exchange ideas and information. It is critical that the ACA remain relevant and vital for all our members, especially in its role in the education and training of young scientists. Today's challenges are great for crystallographers who are in the early stages of their careers. The ACA should help them prepare for the multidisciplinary approach to research that is now the norm for success.

It is the job of the ACA to be an effective research and educational organization for scientists training and working in all fields represented by the ACA. Maintaining balance among the twelve Special Interest Groups in our organization is critical so that we serve researchers and educators interested in all the disciplines represented by the ACA. Toward that end, as Vice President I would work with Program and Session Chairs to further enhance our annual meetings, including seeking additional outside funding so that our programs and workshops can be as rich and varied as possible.

The ACA is a voice for our community of scientists. To the larger scientific community, we must continue to stress the power of diffraction and scattering in structural studies that are important in a wide range of fields.

My seven years serving as the Head of the Department of Molecular and Cell Biology gave me management and administrative experience that I would bring to being a member of the ACA Council. The two years that I served as Chair of the Biological Macromolecules SIG and my stint as Program Chair for the 2006 ACA meeting in Hawaii also give me background that will be valuable if I am elected to the ACA Vice Presidency. I am honored to have been nominated to serve as Vice President. I look forward to the opportunity to join the ACA Council if elected and to fulfilling the responsibilities of the Vice President. I will work hard to help the ACA grow and thrive in the coming years.

Winnie Wong-Ng
Vice-President

Ceramics Division, Materials Science and Engineering Laboratory, National Institute of Standards and Technology, A256 MATLS, 100 Bureau Drive, Mail Stop 8520, Gaithersburg, MD 20899

Education: B.Sc., Chemistry, Chinese University of Hong Kong (1969). Ph.D., Inorganic Chemistry, Louisiana State University (1974) with Steve Watkins; Postdoctoral Fellow/Research Associate/Lecturer in Chemistry Department, University of Toronto, Canada, with Stan Nyburg.

Professional Activities: Local chair, 1998 ACA annual meeting, Arlington, VA; chair/member, ACA Continuing Education Committee (2001-2003); secretary/treasurer, US National Committee for Crystallography (USNCCr, 2000-2003); chair, ACA Warren Award Committee (2005); chair/member: ACA Nominating Committee (2002-2003); co-organizer of four ACA scientific sessions (1989, 1992, 1993, 1998); co-organizer of more than 20 symposia/workshops at various other scientific meetings; chair, Membership Committee, International Centre for Diffraction Data (ICDD, 2001-2004); chair, Ceramics Subcommittee, ICDD (1994-2000); member, ICDD Awards and Scholarship Committees (2004-present); chair, thermoelectric task group, ICDD (2006-present); chair, high-temperature superconductor task group (1994-present); chair, Electronics Division, American Ceramic Society (ACerS, 2005-2006); member, Board of Directors, Applied Superconductivity Conference (ASC), 2008; editor, international report section of Powder Diffraction (1999 - present); guest co-editor, special issue of J. Research of NIST (2001); guest co-editor, special issue of J. American Ceramic Society (2008); *Honors and Awards*: Fellow of ICDD (2001); Fellow of American Ceramic Society (2002); recipient of the Bronze Medal for superconductivity research from Department of Commerce (2002); recipient of the McMurdie Award for significant contribution to the Powder Diffraction File (2004); recipient of the Spriggs Phase Equilibria Award from ACerS (2007); about 260 publications.

Research Interests: Crystallography, crystal chemistry, phase equilibria, structure/property relationships of high temperature materials including complex oxides and metals/alloys; standard reference materials; reference x-ray powder patterns; databases; single crystal and powder diffraction crystallography (x-ray, neutron, and electron); high-temperature x-ray diffraction; modeling; superconductors; thermoelectric materials and other energy-related materials; fast-throughput combinatorial thin film metrology.

Statement: I am very honored to be a candidate for Vice-President in the forthcoming ACA election. ACA is the first scientific organization that I joined when I was a graduate student, and it is an organization that I particularly care about, respect, and 'grew up' with. During my membership years, I have served ACA in several roles such as organizing symposia and serving on ACA committees. In 1998, I enjoyed tremendously the experience of serving as the local chair of the ACA annual meeting in the greater Washington DC area. With that fond memory, I am extremely delighted to have this possibility to serve the ACA again as your Vice-President. As ACA plans its strategies and growth for the years ahead, I would like to share my views concerning the future.

We have just entered a new millennium, and we are facing many new challenges and opportunities. We must keep abreast of the latest technological advances. For example, there are exciting recent developments in the fields of nanoscience and bioscience that require new techniques for characterization. Having worked in

a standards/metrology organization for many years, I recognize the importance of crystallographic metrology. In addition to practicing traditional crystallography, we should encourage the increased use of new scattering metrologies to meet the challenges of nanoscience, such as grazing incidence diffraction and small angle scattering, and reflectivity from thin films. Local structure determination using x-ray absorption spectroscopy combined with x-ray and neutron pair distribution function analysis is another example of where new methods will become more prominent and deserves our increased attention. For biological applications, the phase contrast imaging technique is beginning to play a significant role. We must encourage our members to make the best of the x-ray synchrotron, neutron- and electron-based national research facilities. On the materials front, in addition to maintaining the health and growth of the macromolecular crystallography component of the organization, we also need to advocate and build up the strength of the components that are related to small molecule research, including the complex minerals and materials that are of current technological importance for energy applications. In this way, the harmony between the macro- and small-molecule components of the ACA could be extended to a higher level, with substantial payoff for the crystallographic community as a whole.

The SIGs are vital components of the ACA. We must work closely with them to strive to build a strong and balanced scientific program during the annual meetings that will meet the needs of our members as well as attracting new members. The program should include presentations on state-of-the art techniques, theory, software, and materials of current technological interest. I will work closely with the SIGs to explore opportunities for funding invited speakers necessary to provide us with the best possible meeting content. During these meetings, we should also take the opportunity to increase our visibility by contacting the scientific press to showcase our publications and programs. We should strengthen the special transaction symposia and plenary lectures to reflect state-of-the-art crystallographic research. I will work efficiently to obtain the funding and sponsorship necessary to achieve this, while continuing to maintain individual member subscription fees at a level that provides one of the best values of any professional organization.

With the advent of modern computer technology, there has been tremendous progress in the area of database development. In addition to the availability of macromolecular information from high throughput techniques, a vast volume of other diffraction data will soon be available partly due to the increasing importance of the combinatorial approach in materials research, an area that I am also currently involved in. To be able to access this large volume of diffraction data, various computational strategies and standards are critical for data collection, storage, transport and exchange. Communication and cooperation between creators/producers of crystallographic databases and those responsible for other property databases are important in order to maximize research opportunities for all. We should emphasize the potential of combined use of these databases for enhancing research opportunities to the maximum possible extent.

An effective way to achieve the growth of an organization is through focused membership drives. New members will provide us with new scientific insights and resources. Therefore we need to design strategies to gain new members. There are many scientists who have crystallographic knowledge and are currently participating in other scientific societies, but they are not members of ACA. Many of these societies may also have interests in structural science or crystalline states. We need to cooperate with these organizations to identify potential new members, to ensure that structural data is appreciated, and to raise the profile of our organization. We need to provide potential new members with effective opportunities to join us. The form of cooperation between societies could include joint symposia/sessions and/or cross-links on the world-wide web. We also need to expand membership among our industrial colleagues. Industrial crystallography could be an important component of the association.

I believe a well-planned outreach program is important for the growth and visibility of the organization. In addition to continuing to support research and therefore education, and to meet the needs of membership, we need to increase our outreach to Central and South America. We should also facilitate educational opportunities for the general public, for example by encouraging our members to give talks about crystallography at local high schools. We can also encourage teachers from local schools to teach crystallography by inviting them to attend selected sessions on crystallographic education during the annual meetings. To do this we need to develop appropriate publicity leaflet materials.

Our institutional health relies heavily on continuing crystallographic education. We must continue to build upon this important aspect for both the young members as well as for the more established professionals. It is our responsibility to ensure the strength and skills of the next generation of crystallographers by providing them with the necessary education and training. We will strive to increase resources for supporting attendance of more young people at ACA annual meetings. We will investigate possible ways of establishing scholarships for crystallographic studies. We will make sure our annual meeting program will continue to meet the needs of our members by providing ample networking opportunities and mentoring by senior members. We must also continue to support and encourage the ACA for the macromolecular and small molecule summer schools.

If possible, I suggest that ACA make available the information from science policy makers to the crystallographic community. We should establish efforts to help influence public policy, particularly as related to the support of national resources such as the synchrotron, neutron and electron research facilities, as they are vitally important to many of our members. We will investigate the possible creation of a mechanism to bring the members' concerns to the attention of the policy makers. We should also support efforts to increase public funding of all components of crystallographic research.

I have a combined total of 30 years scientific experience. I believe I can bring to this office an appreciation for the diverse and exciting field of crystallography. If honored with your election to the position of Vice-President, I pledge to commit my best abilities to fulfilling the responsibilities of the office. I recognize that the vice president position comes with many key

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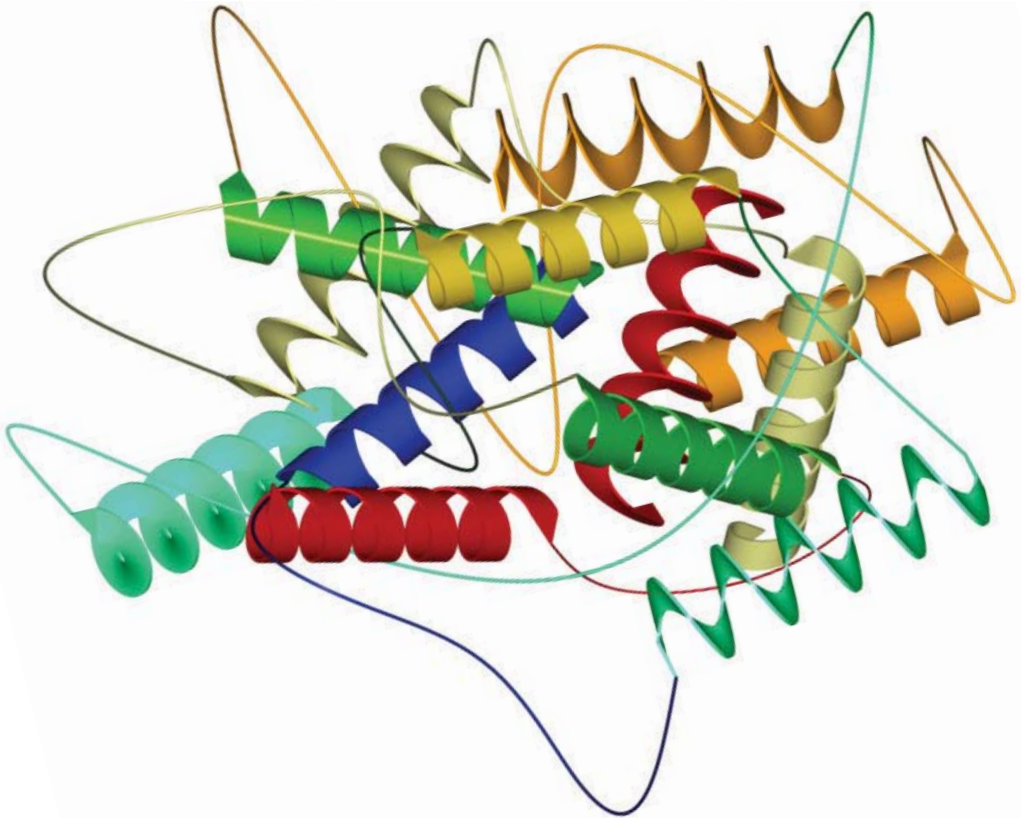

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responsibilities. If elected as your Vice-President, I would apply the experience that I have gained in working at academic, industrial and government institutions to serve the ACA. I would solicit advice from other ACA officials, ex-officials, and members. Together with the council members, I would strive for the continuous prosperity and growth of our organization, and the steadfast advancement of the field of both macromolecular and small molecule crystallography.

Patrick Loll - Secretary

Professor of Biochemistry and Molecular Biology, Drexel University College of Medicine, Philadelphia, PA, USA

Education: B. Ch. E. Chemical Engineering, Catholic University of America (1981); Ph. D., Biophysics, Johns Hopkins University (1989); Post-doctoral, University of Chicago (1989-1995).

Professional Activities: Co-editor, *Acta Crystallogr. F*; Member ACA since 1988; ACA Pauling Prize committee (1998, 2002); Member, Protein Society, Biophysical Society, and American Chemical Society; Instructor and advisory panel member, NSLS Workshop on membrane protein crystallization.

Research Interests: Structural basis of antibiotic activity; structure-based drug design; membrane protein structural biology; macromolecular crystallization.

Statement: The ACA has been a phenomenal resource for me over the last two decades, and I would be delighted to support its continued success by discharging the duties of the Secretary. In addition to acting in an organizational support role, the Secretary is a member of Council, and as such can influence the ACA's future direction. I feel prepared for this role, since 1) My own research places me within the burgeoning structural biology "wing" of the ACA, and I have developed a keen appreciation for the tremendous new challenges facing structural biology in the post-genomic era; and 2) During my career I have also been lucky enough to be exposed to many other aspects of diffraction, including chemical crystallography, methods development, solution scattering, and crystallographic education. These experiences gave me an appreciation for the extraordinary diversity and scope of the disciplines falling under the ACA's umbrella, and I believe it is critical that the ACA continue to represent the broadest possible spectrum of interests. As Secretary, I would be honored to would work diligently toward this goal.

Carrie Wilmot - Secretary

Associate Professor with Tenure, Department of Biochemistry, Molecular Biology & Biophysics, University of Minnesota, Twin Cities; Director of the Kahlert Structural Biology Laboratory, University of Minnesota.

Education: BSc Hons Biophysics, University of Leeds, UK (1986); PhD Biophysics, Birkbeck College, University of London, UK (1989), advisor Janet M. Thornton; Cancer Research Institute Postdoctoral Fellow, The Scripps Research Institute, La Jolla, CA (1989-1992) with Ian A. Wilson; Research Fellow, University of Leeds, UK (1992-1999) with Simon E.V. Phillips.

Professional Activities: European Molecular Biology Organization (EMBO) Short Term Fellowship, Uppsala University, Sweden (1997) with Janos Hajdu; Director of Facilities, North of England Structural Biology Centre (NESBiC), U.K. (1999-2001); Paul D. Saltman Memorial Award, Metals in Biology Gordon Research Conference (2006); Margaret C. Etter Early Career Award, ACA (2006); Conference organizer (3rd Int. Symposium on Vitamin B_6, PQQ, Carbonyl Catalysis and Quinoproteins, Southhampton, U.K. April 14-19, 2002); Session organizer (Glasgow Protein Structure Workshop, 1998, 1999, 2000; IUCr 1999, 2005; Int. Conf. on Biological Inorg. Chem., 2005; BioMac SIG sponsored sessions, ACA Meeting 2008); Chair-Elect (2007) & Chair (2008), ACA BioMac SIG; Member (2005-2008) & Chair (2008-present), NIH Advisory Comm. to BioCARS sector, APS; Member (2007-present), Margaret C. Etter Early Career Award Nomination Committee, ACA; Editorial Boards (*J. of Biological Inorganic Chemistry* (2006-present); *J. of Biological Chemistry* (2008-present)).

Research Interests: Structural enzymology of metal and organic cofactor containing enzymes. Combining macromolecular x-ray crystallography with various single crystal spectroscopies. Freeze trapping catalytic intermediates for monochromatic x-ray diffraction experiments, in addition to developments in Laue diffraction.

Statement: I am honored to be standing for the position of ACA Secretary. I have been a member of the ACA since 1999, and I am currently the Chair of BioMac SIG. As Chair, I have had the pleasure of putting together the BioMac SIG sponsored sessions for the Knoxville meeting, which has given me insight into how the ACA functions. The position of Secretary primarily requires organizational skills. In my current position as Director of the Kahlert Structural Biology Laboratory at the University of Minnesota, and in my previous position as Director of Facilities of North of England Structural Biology Centre (NESBiC) in the UK, I gained considerable experience in organization. I have also organized an international symposium, and Chaired sessions at multiple conferences. If elected I will put my organizational skills to good use in promoting informational dissemination and exchange within the ACA community.

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Alicia Beatty - Communications

Associate Professor: Department of Chemistry and Biochemistry, University of Missouri-St. Louis, St. Louis, MO 63121.

Education: B.S. Chemistry, UM-St. Louis (1989); Ph.D. Chemistry, Washington University in St. Louis (1994).

Professional Activities: Previous service for ACA: Chair, Service SIG (2003); Chair, Small Molecule SIG (2006); Organizer, *Transactions Symposium* on *Crystals in Supramolecular Chemistr*y (2004); Other Service: Organizer, Symposium on Crystal Engineering, Southern Style for the Southeast Regional ACS meeting (2007), Member of the International Advisory Board for CrystEngComm (2006-present), Member of the Strucural Chemistry Commission for the IUCr (2006-2009).

Research Interests: Inorganic/organic supramolecular and solid-state materials chemistry, crystal engineering.

Statement: Thank you for considering me for the ACA Communications Committee. I've enjoyed my past service to the ACA, and would look forward to a new challenge as a member of this standing committee. If elected, I will do my best to help coordinate electronic and printed publications of the ACA, to prepare reviews of crystallographic research, and to facilitate the development of articles on "hot topics" and/or on historically-significant people, places, and happenings. I will faithfully execute all other duties associated with the ACA's interactions within the ACA and with the scientific community at large.

Thomas Proffen - Communications

NPDF Instrument Scientist, Lujan Neutron Scattering Center, LANL, MS H805, Los Alamos, NM 87545.

Education: PhD in crystallography at the University of Munich, postdocs at the Australian National University and Michigan State University.

Professional Activities: Co-editor for *Zeitschrift fur Kristallographie*, member of the executive committee of the instrument advisory team for the single crystal diffractometer TOPAZ under construction at the Spallation Neutron Source, past chair of the Neutron and current chair of the Powder Diffraction SIG.

Research interests: Study of disordered materials using total neutron and x-ray scattering applied to exotic oxides, geomaterials and more recently hydrogen storage materials. I started my career analyzing single crystal diffuse scattering from inorganic materials and over time became involved with atomic pair distribution function analysis to study similar disordered materials using powder diffraction. As an instrument scientist at NPDF at the Lujan Center, my technical interests include software development for data reduction and modeling as well as getting the PDF technique 'out there'.

Statement: Being a crystallographer (I indeed have a PhD in crystallography) by education, I joined the ACA as soon as I came to the US about 9 years ago. One issue close to my heart is bringing a notion of what and how important crystallography is to the wider public, to schools and to the colleagues in the next building. On more than one occasion when asked my profession, my reply 'I am a crystallographer' resulted in being asked abou the healing powers of a particular stone, so there is a long way to go. I remember attending the IUCr meeting in Seattle and, in particular, listening to the panel discussion by several Nobel prize winners, all related to crystallography. Even I was impressed. I see the function of the ACA Communications Committee as key to providing a united voice to politicians, funding agencies and the public and, if elected, I will work as hard as I can to achieve these goals.

Cora Lind - Data and Standards

Associate Professor, Department of Chemistry, University of Toledo, Toledo, OH.

Education: Prediploma, 1996, Bergische Universität Wuppertal; MS 1999, PhD, 2001, Georgia Institute of Technology.

Professional Activities: Member ACA, ACS, MRS, PDS; Symposium Organizer, Pittsburgh Diffraction Society Meeting (2004); U.S. National Committee for Crystallography (2007-2009); Chair, ACA Powder Diffraction SIG (2008); Instructor, ACA Crystallography Summer Course (2008). Etter Award (2007).

Research Interests:Structure-property relationships in solid-state materials, x-ray and neutron powder diffraction, Rietveld analysis, structure determination from powder data, non-ambient diffraction (low+high temperature, high pressure),

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phase transformations as a function of temperature, pressure and composition.

S*tatement:* Crystallography has been transformed from an "experts only field" to a tool open to many researchers. A major driving force of this change has been the incredible increase in computing power over the past decades, which makes characterization of simple structures a routine task that can often be accomplished by simply "pushing buttons". With this increase in user base and computing power comes the responsibility for our community to provide databases and standards that allow users of crystallography to ensure the soundness of their data even if they are not "experts in crystallography" in the traditional sense. This requires easy access to data and standard procedures.

In my opinion, there are several areas related to data and standards that would benefit a number of users if the following improvements could be implemented: 1) The current "site licensing" policies of many database vendors is very restrictive, and can be counterproductive in an academic setting. Many companies require multiple copies of a site license to be installed in the same physical building to be eligible for reduced pricing on additional licenses. This is not feasible at most North American universities, especially with new interdisciplinary buildings that often spread members of the same department across several buildings. Some companies have started to explore web based licenses, which require a login and limit the maximum number of concurrent users. Such options should be encouraged for all database products. 2) To facilitate user education about databases and software, database/software companies should be encouraged to grant short-term educational free-of-charge licenses (e.g., 2-4 week period for class use by instructors). This is already common policy for some analysis programs, but rare for databases. If web based copies for databases existed, instructors could use this mode of access for licenses available at their institution, or apply for a short term access code for classroom use through the respective company's server. 3) Diffraction standards for diffractometer alignment under ambient conditions are readily available through NIST and other vendors. However, standards for non-ambient experiments are much less explored, and knowledge about standards and appropriate calibration procedures is less widespread. Many users of variable temperature options on in-house diffractometers rely on thermocouple readout for their non-ambient experiments. This can lead to significant errors in temperature estimates. "Standard procedures" are rare to non-existent.

If elected, I would work with the Committee and the ACA to encourage database and software companies to explore the above outlined options that allow broader access and education of users. I would also work with experts in variable temperature diffraction to develop suggestions for standardized procedures (including *in situ* temperature standards) for non-ambient experiments for different types of variable temperature stages.

John Rose - Data and Standards

Associate Professor of Biochemistry and Molecular Biology, University of Georgia, Athens, GA 300602. Assistant Director, Southeast Regional Collaborative Access Team, Advanced Photon Source, Argonne National Laboratory.

Education: Ph.D. (1980) in Physical Chemistry, Rutgers University, Newark NJ with Roger A. Lalancette, B.A. in Chemistry (1974) Benedictine College, Atchison KS.

Professional activities: Research Associate, Dept. of Crystallography University of Pittsburgh (1980-86), Consultant, Dept. of Surgery, University of Pittsburgh (1984-86), Manager, Shared X-ray Diffraction Facility, University of Pittsburgh (1986-95), Research Assistant Professor, Dept. of Crystallography, University of Pittsburgh (1989-95), Consultant Protein Data Bank (1989-99), Visiting Specialist, Institute of Molecular Biology, Academia Sinica, R.O.C. (1990-92), Adjunct Asst. Professor Dept. of Crystallography, University of Pittsburgh (1995-99), Assoc. Research Scientist, dept. of Biochemistry & Molecular Biology, University of Georgia (1995-2002), Editorial Board, Protein Data Bank, Brookhaven National Laboratory, Upton NY (1996-99), Asst. Director Southeast Collaborative Access Team, Advanced Photon Source, Argonne National Laboratory (1999 - present), Director and Co-PI Bioinformatics Core, Southeast Collaborative for Structural Genomics (2000-07), Senior Research Scientist, Dept. of Biochemistry & Molecular Biology, University of Georgia (2002-04), Associate Professor Dept. Biochemistry & Molecular Biology, University of Georgia. Member American Crystallographic Association, Local organization ACA Annual Meeting, Pittsburgh (1992), Poster Chairman ACA Annual Meeting, Pittsburgh (1992), Tutor ACA Summer Course for Crystallographers (1992-2001), Lecturer ACA Summer Course for Crystallographers (1997-2001), Member APS Users Organization Steering Committee (2001-04), Chairman APS MC Proposal Review Panel (2006-). Served as a member of 13 NIH review panels (2000-present).

Research interests (1) x-ray structural biology focused on proteins of the mitochondrial intermembrane space import pathway and structure assisted vaccine and therapeutic design. (2) Methods development related to Direct Crystallography including soft x-ray SAS data collection/phasing and Sulfur-SAS structure determination. (3) Signal Based Data Collection - an expert system for fully automated synchrotron data collection and phasing.

Statement: I am happy to accept this nomination to the Data and Standards Committee. Being trained as a small molecule crystallographer and having spent over 25 years as a practicing protein crystallographer, I know the importance of reliable and validatable data standards. This is especially important today as the field of structural biology is expanding

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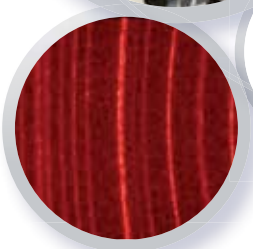

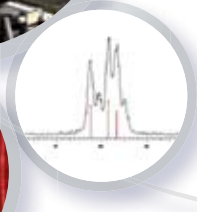

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at a phenomenal pace with over 50,000 structures in the Protein Data Bank. I also believe that my experience as a consultant and annotator for the PDB for almost 10 years has given me a unique perspective on data validation and data standards, which should be of benefit to the ACA. Finally, as a researcher and teacher who uses structural information provided by others, it is important that this information be reliable and complete.

There are several areas that need our attention: (1) Software development - I believe all federally supported software development projects should be open-source and all software adequately documented so that others can modify the code to add features or address local concerns.

(2) Data formats - there should be a standardization of the image and reflection file formats. Instrument and software producers should be encouraged to produce image files in imageCIF format for long-term compatibility.

(3) Raw data - raw image files related to the refined structure reported in the literature should be publicly archived in a standard and supported format.

(4) Web tools - There has been an explosive growth of web tools for structure validation and analysis both for small molecules and macromolecules. However, it is important that these tools/databases be well documented, maintained and updated, if needed, to reflect the ever-growing PDB and other databases.

(5) Training - as more and more researchers are adding structural studies to their research program it is imperative that these investigators and their students have a solid understanding of the software used in the analyses and potential sources of error, both in the data itself and in the resulting structure.

If elected, I would work with the Committee, the ACA, and others to help address these areas. I would also encourage the ACA to continue activities such as symposia, workshops and the ACA summer schools aimed at training the next generation of crystallographers.

Allen Hunter - Continuing Ed.

Director of the YSU-PUI Undergraduate Diffraction Consortium, YSU Structure and Chemical Instrumentation Center, YSU-S&CIC, Professor of Chemistry, Department of Chemistry, Youngstown State University One University Plaza, Youngstown, Ohio 44555-3663

Education: B.Sc., University of British Columbia (1981); Ph.D., University of British Columbia (1985); Postdoctoral Fellow, Australian National University (1986) and University of Alberta (1987).

Professional Activities: Assistant Professor, University of Alberta (1987-1992); Associate Professor, Youngstown State University (1992-1998); Full Professor (1998-pressent). Founder and director of the YSU-PUI Undergraduate Diffraction Consortium which employs local and remote diffractometer control to give access to the four diffractometers at Youngstown State University to faculty and students of other Predominantly Undergraduate Institutions. Active in the development of crystallographic education materials, especially those designed for undergraduate students. Member of the editorial board of the *Journal of Chemical Crystallography*. Organizer of, and presenter to, crystallographic education symposia at recent ACA and ACS national meetings. DoD, NSF, and ACS-PRF grantee and proposal reviewer. Member of ACA, BCA, PDS, ACS, and CUR. This year, I am Co-Chair on the NSF Chemistry Division's Workshop on CyberInstrumentation.

Research Interests: Synthetic materials chemistry, chemical and crystallographic education, applications of x-ray methods to structure determination, and CyberTechnology. While I was primarily trained as a synthetic organometallic chemist, over the last decade I have become increasingly active in crystallography and allied analytical/structural techniques. The central focus of my current research is the development, testing, and distribution of a new set of software/IT/hardware tools for the remote operation of scientific and engineering instruments. These tools are optimized for use with large numbers of different instruments in dynamic networks, for a large dynamically changing user base (many of whom are relative novices), and for the maximum achievable automation in both data collection and analysis and in the network overhead functions (i.e., user authentication, data distribution & archiving, billing, etc.).

Statement: While the ACA must continue to play a central role in the education of professional crystallographers, I believe that it is *equally important* for the ACA to play a central role in developing, evaluating, and disseminating educational materials aimed at non-specialists. This reflects the reality on the ground that non-specialists are increasingly involved in crystal structure determinations. It also provides us with opportunities to show off the beauty and power of our technique and to recruit future crystallographers. To this end, if I am elected to the continuing education committee, I will concentrate my efforts on working with other committee members and the larger community in identifying, evaluating, and distributing exemplary materials, modules, and courses that can be integrated into non-crystallographic courses by both expert crystallographers and those earlier on the learning curve. In addition, I will work with the committee and others to increase the awareness in the community of funding opportunities to support these efforts and at funding agencies of the need for such grants.

Bill Ojala - Continuing Ed.

Assistant Professor, Department of Chemistry, University of St. Thomas, St. Paul, MN.

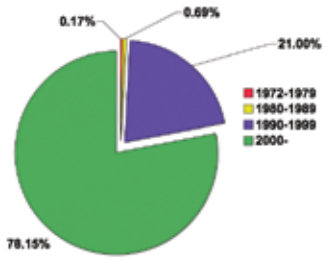
Education: B.S. College of Great Falls, Great Falls, MT (1977), Ph.D. University of Minnesota, Minneapolis, MN (1986).

Research Interests: Packing preferences of isomeric small molecules; phase transitions in small-molecule solids; crystal structures of monosaccharide derivatives.

Statement: Few other scientific fields have undergone so dramatic a transformation within the time span of the average research career as crystallography. Keeping pace with this spectacular rate of change makes the field both challenging and enjoyable to those of us who have the opportunity to participate in it. Staying current with these changes is not always easy for those of us who work in primarily undergraduate institutions. On the other hand, we who work in small liberal arts colleges and universities while trying to remain in touch with major developments in our field are perhaps uniquely mindful of the importance of lifelong learning; this is a value that our particular academic environment especially encourages us to share with our students and to apply to our own scientific practice. In seeking a position on the Continuing Education Committee, I hope I can be especially helpful to faculty and staff from smaller institutions who wish, like I do, to be actively engaged with the rapid progress that continues to be made in our science.

PDB Archives 50,000th Structure

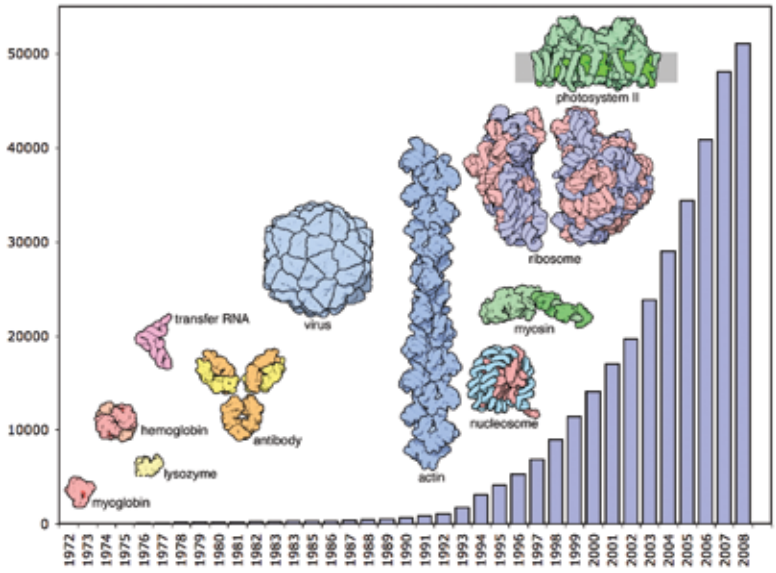
The PDB archive reached a significant milestone in its 37-year history this past spring. The 50,000th molecular structure was released into the archive on April 8, joining other structures vital to biology, medicine, and education.



The worldwide Protein Data Bank (wwPDB) is estimating that the size of the PDB archive will triple to 150,000 structures by the year 2014.

This chart shows the percentage of structures released into the PDB archive in the decade of deposition. Since the year 2000, almost 40,000 structures have been deposited.

The wwPDB has seen the archive double in size since 2004. The PDB archive was founded in 1971 with seven structures at Brookhaven National Laboratory. Today, the wwPDB receives approximately 25 new experimentally-determined structures from scientists each day for inclusion in the archive. These data are checked and processed by annotators located around the world.



Structures available in the archive by year

More than 10 million files - 2 Terabytes of data - are downloaded from the PDB archive at ***ftp://ftp.wwpdb***.org each month by an average of 7,000 unique visitors. Even more data are downloaded from wwPDB mirrors at PDBj and PDBe. Users include structural biologists, computational biologists, biochemists, and molecular biologists in academia, government, and industry as well as educators and students.

wwPDB members also provide a variety of ways to explore PDB data by developing online databases that promote searching, reporting, and visualizing structures. They will demonstrate their latest developments at the IUCr meeting in Osaka. For information about the wwPDB, please see ***www.wwpdb.org***.

The wwPDB consists of organizations (RCSB PDB, PDBe, PDBj, and BMRB) that act as deposition, data processing and distribution centers for PDB data. The mission of the wwPDB is to maintain a single Protein Data Bank archive of macromolecular structural data that is freely and publicly available to the global community.

Christine Zardecki

The Molecule of the Month at the RCSB Protein Data Bank Marks its 100th Edition

In the decades since its inception, the Protein Data Bank has grown from a specialist resource for crystallographers into the world's primary window into the discoveries of structural molecular biology. The PDB has grown and diversified, now including over 50,000 structures ranging in size from hormones to ribosomes, and the user community has continued to grow and diversify along with it (see page 33). Today, the PDB is used by crystallographers, spectroscopists and microscopists as their primary archive of results. It is used by computational biologists as the source of coordinates for further study. It is used by the wider community of biologists to add structural insight to their results. And more and more it is being used by students, educators and the lay audience to explore first-hand the current topics in biomolecular science. I began work on the Molecule of the Month eight years ago to help make the often-daunting resources of the PDB more friendly and accessible.

The Molecule of the Month (MOM) presents a new biomolecule each month. Since the goal of the column is to generate excitement and entice visitors to explore the PDB, I try to choose subjects that have relevance to health and welfare, or that may be familiar in some aspect of our daily lives. The column presents a few structures related to the subject, highlighting the structure and function of the molecule and then showing how they affect our health and welfare. The column ends with a page entitled "Exploring the Structure" that guides the visitor through the structural aspects of one particular PDB entry and provides an entry point for further exploration.

After 100 installments, I have barely scratched the surface of what is available. A few examples of structures highlighted in past installments are included here. You can visit the Molecule of the Month at the RCSB PDB site at ***www.rcsb.org*.**

Fig 1. The adrenergic receptor was presented as the 100th installment of the MOM. This image, shows the bound carazolol molecule, but omits the lysozyme chain that was engineered into the protein to assist with crystallization. PDB entry ***2RH1***. ***Fig 2.*** The ribosome was presented in the first year of the MOM, soon after the first structures were released. It is probably time for an update on this subject, since at the time the only structure of the large subunit included only alpha carbon positions for the proteins, and many amazing structures of functional complexes of ribosomes with the machinery of translation are currently available. PDB entries ***1FFK*** and ***1FKA***. ***Fig 3.*** Of course, myoglobin was the first installment of the MOM. PDB entry ***1MBN***. ***Fig 4.*** For the 50th installment of the MOM, I explored the structures of all 10 glycolytic enzymes. The final protein in the pathway, pyruvate kinase, is shown here. PDB entry ***1A3W***. ***Fig 5.*** In response to requests from visitors, the MOM now includes interactive Jmol images on the final page. This molecule is the KaiC circadian clock protein, presented as the 97th installment. PDB entry ***2GBL***. (**See page 18: *RefleXions Inside and Out* for references**).

David S. Goodsell Department of Molecular Biology The Scripps Research Institute

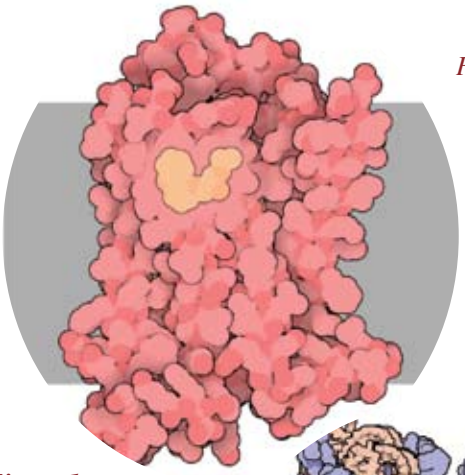


Figure 1

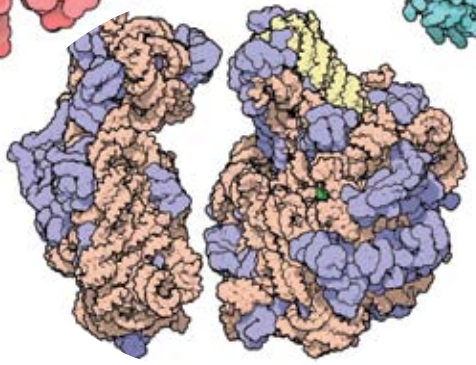
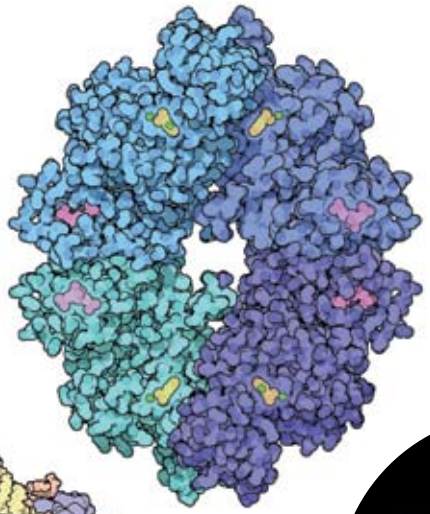


Figure 2

Figure 4



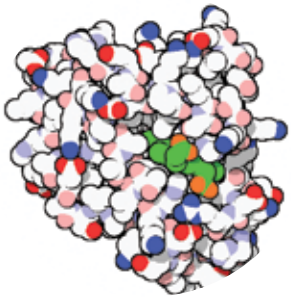


Figure 3

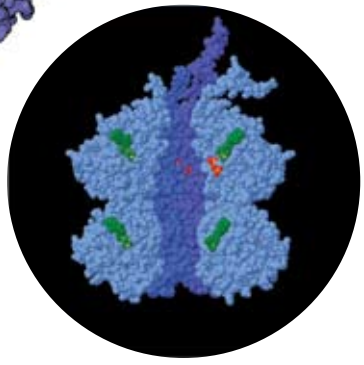


Figure 5

2008 Travel Award Winners

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Changrui Lu
Cornell University
David Critton
Brown University
Robert Spitale
University of Rochester
Marianne Lee
Ohio State University
Helen Rho
Rochester Institute of Technology
Jin-Yi Zhu
University of Georgia
Theresa Detrie
Virginia Tech
Matthew Hudson
Groningen University (Netherlands)
Liangming Hu
Virginia Tech
Paul Tongwa
New Mexico Highlands University
Kristin Wunsch
Hauptman-Woodward Med Res Institute
Breann Brown
Brown University
Louise Dawe
Memorial University (Canada)
Karen Mulfort
Northwestern University
Clare Yannette
Georgetown University
Elinor Spencer
Virginia Tech
Marta Dabros
Worcester Polytechnic Institute
Ilana Goldberg
Georgetown University
Julio Cesar Silva
Physics Institute - UNICAMP (Brazil)
Efstratios Mylonas
EMBL-Hamburg (GermanY
Sterling Cornaby
Cornell University
Xuerong Liu
University of California, San Diego
Christina Capacci
Georgetown University

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Etter Early Career Award

Radu Custelcean
Oak Ridge National Laboratory

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Alexey Amunts
Tel Aviv University
Fiber SIG
Olga Antipova
Illinois Institute of Technology
Materials Science SIG
Xuerong Liu
University of California San Diego
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Matthew Hudson
Syracuse
Powder Diffraction SIG
Daniel Mitchell
University of Tennessee
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Calendar of Future Meetings

AUGUST 2008

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

SEPTEMBER 2008

18-22 **11th European Powder Diffraction Conference**. Warsaw, Poland. *www.epdic-11.eu/.*

20-24 **ICSG 2000: International Conference on Structural Genomics**. Oxford. UK *www.spine2.eu/SPINE2/ISGO/index.jsp.*

OCTOBER 2008

15-17 **Modern Trends in Neutron Scattering Instrumentation.** Munich, Germany. *www.jcns.info/Workshop/.*

19-26 **EMBO Practical Course in Solution Scattering**, EMBL, Hamburg, Germany. *www.embl-hamburg.de/workshops/2008/EMBO/.*

NOVEMBER 2008

9-14 **EMBO World Lecture Course - Recent Developments in Macromolecular Crystallography.** Pune, *India. cwp.embo.org/wpc08-02/index.html.*

16-20 **SARX2008: Latin american Seminary of Analysis by X-Ray Techniques.** cab Frio, Rio De Janeiro, Brazil. *www.lin.ufrj.br/sarx2008/*.

APRIL 2009

5-8 **The 19th West Coast Protein Crystallography Workshop**. Asilomar, CA The schedule will be dominated by oral presentation by students and postdocs, *wcpcw.org.*

MAY - JUNE 2009

30-3 **Small Molecule Workshop at the 92nd Canadian Chemistry Conference.** Hamilton, ON, Canada.

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

9-14 **XXV European Crystallographic Meeting.** Istanbul, Turkey.

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

JULY 2010

24-29 **ACA Meeting - Chicago, IL.**

MAY-JUNE 2011

28-2 **ACA Meeting - New Orleans, LA.**

JULY 2012

21-26 **ACA Meeting - Boston, MA.**

ACA Annual Meeting
Toronto -
July 25-30, 2009
Pre-Meeting Travel Tips

Visa/Passports: You should plan to have a valid passport to enter Canada. US and European nationals generally do not need a visa (you can check here to be sure *www.cic.gc.ca/english/visit/visas.asp*). ***Everyone*** will be required to have a valid passport to return to the US by air **(even US citizens).** It is likely that this will apply to land crossings as well by July, 2009.

***Note: It can take time to process passport applications so get an early start*!** Non-US nationals working in the US are strongly advised to understand fully the travel restrictions associated with their US Visa (especially re-entry). Check the ACA website for more details (*www.amercrystalassn.org).*

Currency: Canada uses the Canadian Dollar. As of May, 2008, the Can$ is essentially at parity with the US$. US currency can be exchanged for Canadian freely at banks and hotels. Many tourist services and shops will accept US cash directly. Bank cards will probably work in most ATM machines, and credit cards are accepted widely.

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