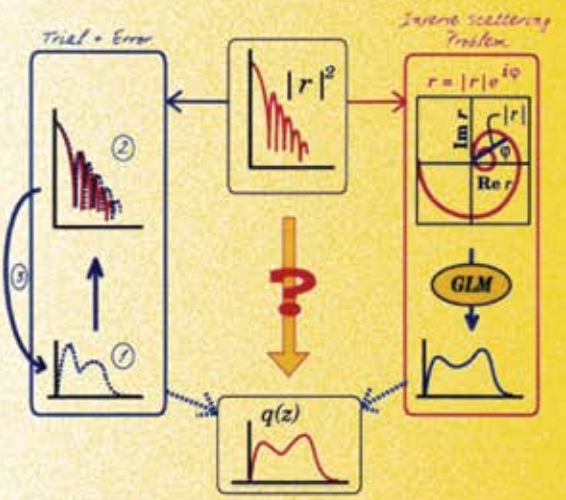
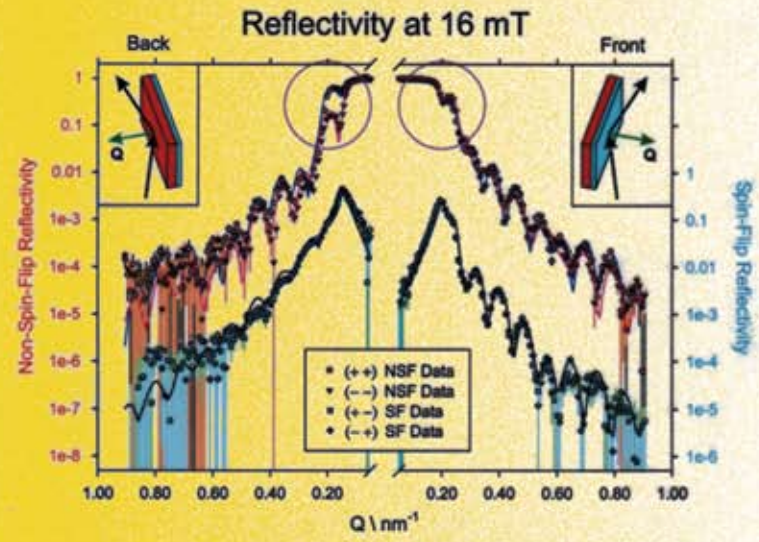
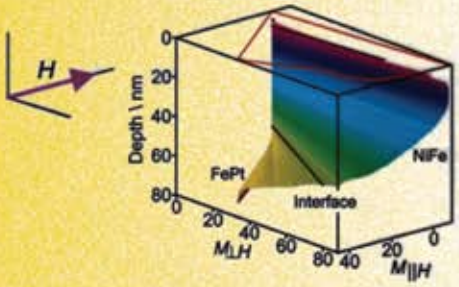
American Crystallographic Association

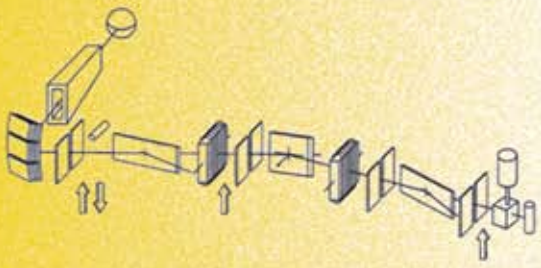
Reflections

Number 1
Spring, 2006









Neutron Reflectivity

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American Crystallographic Association

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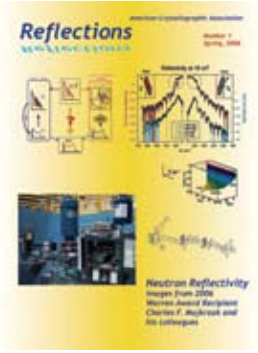
*see page 9 for notes on our new name and for new logo possibilities



Cover: **Images from Warren Award Recipient Charles Majkrazk and his colleagues; see page 25.**

ACA HOME PAGE: **hwi.buffalo.edu/ACA/**

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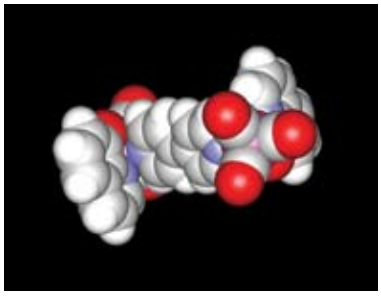

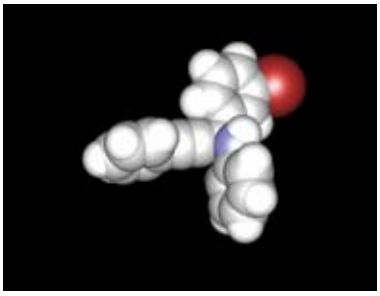

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Rigaku

At the outset, let me thank my predecessor Louis Delbaere for the excellent way he led the ACA, and welcome our new V.P. Alan Pinkerton to the fold. At this time it is also appropriate to thank those who contribute to the smooth functioning of the organization, and much credit is due our Chief Executive Officer, Bill Duax, and our Chief Financial Officer, S.N. Rao as well as our *Newsletter* Editors Judy Flippen-Anderson and Connie Chidester. Because these people and our ACA Council; SIG officers; Standing Committees and Local and Program Chairs are all volunteers who lead very busy lives apart from the ACA, very little would get done without our competent professional staff. We are grateful to our Director of Administrative Services, Marcia Colquhoun, and to Patti Coley, Erica McMehan and Jennifer Curtice for their invaluable services.

Sadly, with this issue we must also mourn the passing of two ACA colleagues, former ACA President Robinson Burbank and Reuben Rudman, who was a long time loyal member.

At our Annual Meeting in Honolulu, Hawaii, July 22-27, 2006, we will have a unique opportunity to discuss science in an idyllic setting, and I hope that many of you will take advantage of this rare opportunity. Hawaii was selected partly with the intention of attracting crystallographers from other Pacific Rim communities, as well as, hopefully, representation from Latin American countries. To make it easier for people to attend this meeting, we have made a special effort to negotiate reduced hotel rates for students and postdocs; those interested in taking advantage of this option are urged to check out: **xray.chem.ufl.edu/aca2006/accommodations.html** as soon as possible. Our sincere thanks to Local Chairs Charles Simmons and Karl Seff and Program Chair Judy Kelly for their tireless efforts toward making this meeting a big success.

The *Transactions* symposium in Hawaii will be on Neutron Crystallography: "The Future of Neutron Crystallography: Smaller Crystals, Larger Molecules" which should raise our awareness of exciting opportunities that will soon "change the landscape" as far as single-crystal neutron diffraction is concerned. We expect that the new ultra-high-intensity Spallation Neutron Source (SNS) currently being built at Oak Ridge, Tennessee (and other similar facilities under construction in other parts of the world) will, by greatly reducing the size of crystals needed and the time required for a neutron analysis, do for neutron diffraction what synchrotrons have done for x-ray data collection. There will also be symposia to honor the 2006 Buerger and Warren Award winners Helen Berman and Charles Majkrzak, and the Etter Early Career Awardee Carrie Wilmot. The symposia organizers and some details about the exciting workshops planned are on page 35.

Please be aware that the nomination deadlines for the 2007 Fankuchen, and Trueblood Awards to be presented at next year's Salt Lake City Meeting are coming up soon (May 1, 2006). (The Etter Award deadline is September 1st.) See **hwi.buffalo.edu/ACA/Awards.htm** for details about these awards and forms. Finally, the sites and chairs of some future meetings have been decided. For the 2007 meeting in Salt Lake City, Chris Hill will be the Local Chair and Jill Trewhella the Program Chair. In 2008 at Knoxville, Jason Hodges will be Local Chair and Paul Butler and Dean Myles will share the Program Chair responsibilities. To all of these individuals who have graciously agreed to donate their time and services, we owe a big "Thank You"!

Bob Bau

Guest Editorial: Comments on the State of Science Education

by Miriam Rossi, Mary Landon Sague Professor of Chemistry, Vassar College

Photo courtesy of Christine Zardecki, PDB.

Diminishing standards for science and math in pre-college education as well as the declining numbers of students entering a career in science are the subject of many current news articles. The National Academies of Science issued a 2005 report (**books.nap.edu/catalog/11463.html**) describing this dismal state of affairs. Moreover, this trend is not restricted to the US and it has far reaching implications since many technical professions have a scientific basis (e.g., mechanic, nurse, plumber). As scientists, we need to ask ourselves what can be done to stop this apparently gloomy outlook which foretells a future with few scientists and numerous scientifically uninformed lay persons. Some reflection is in order about this situation. We need to ask how scientists are portrayed and how they are viewed; we need to investigate how math and science are taught in the K-12 world and at the introductory university level. Finally, policy decisions at all levels need to be made that reverse this tendency toward poor science education and negative public perception.

Children are (and always were) excited by science and technology; nowadays, they are exposed to it at an increasing level as our society becomes more technological. Besides, many of the movies they are most attracted to – from Harry Potter to the Star Wars series - promote a positive image of science and technology. It would appear that the conditions are right for rising awareness towards science. Why, then, are these children not overwhelmingly seeking careers in scientific and technological fields?

How is science and math taught? First, we need to be aware that the K-12 world is rapidly changing. As our society evolves, so does what it means to be a child and to grow up. Children have easy access to computers, the internet, and electronic games. Play-dates frequently have to be arranged and physical activity needs to be scheduled. While the health consequences of physical

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inactivity have been addressed, the intellectual outcome of such a lifestyle has received less attention.

Very young children are naturally curious and need little encouragement in questioning their environment and developing an analytical outlook. Nonetheless, our children are avid consumers of digital electronics from quite a young age. Increasingly, play then becomes not only more solitary but also a two-dimensional activity (watching TV, movies or playing with video games); we need to know how this affects a child's spatial analysis and experimental outlook. Play needs to be recognized as a three-dimensional activity; it leads to scientific curiosity. Bart Kahr at the University of Washington has noted that the concept of kindergarten was founded on ideas relating to spatial understanding through crystallographic principles **depts.washington.edu/chemfac/kahr_pubs.html.**

The basic tenets of science can be taught in a fun and unstressed manner that enhances learning. When my son was in elementary school, his school PTA brought in a two-person show, Mr. Fish and Lisa Lou, (**encoreperforming.com/mf.htm**) who are professional actor-clowns that presented the children with chemistry and physics facts. This show generated excitement, questions, and a desire to learn more; it did more to instill an interest in science than most carefully planned lectures. Programs like this one highlight the fact that channeling curiosity is the hallmark of a scientist. Recognizing this needs to be an objective of school curricula since this curiosity can be diminished easily and in some cases almost decimated.

Teachers themselves are not working under ideal conditions. There are not enough science teachers, and at times those whose specialty is far removed from science such as English or Reading are required to teach science. With the adoption of the No Child Left Behind Act, teachers have an increased workload and added pressure to ensure students pass state qualifying exams. Therefore, the guided inquiry aspect of teaching is neglected in favor of implementing the approved school board curriculum that will guarantee a school's success in statewide exams. Children are taught fairly complex scientific principles at an early age, and asked to memorize them. For example, one of the science modules in the 6th grade science curriculum in Dutchess County, New York, has children memorize the names of bones, muscles and tendons in the human body. Consequently, students are sometimes overwhelmed by these exercises, resulting in stress ("I try my best but it's not good enough.") and decreased motivation to attend school. Clearly, this is not how we want our 11 year-olds to be thinking.

Are we turning off our young students to science by taking inquisitiveness away and replacing it with rote memorization of facts that are not hierarchal? Would it not make sense for there to be a national curriculum incorporating age-appropriate scientific principles obtained from a panel of experts such as the National Academies of Science? Such a program ensuring that our students are scientifically literate could be modeled after the successful college chemistry department official recognition plan of the American Chemical Society, (**chemistry.org/portal/a/c/s/1/acsdisplay.html?DOC=education\cpt\guidelines.html**). The ACS accredits chemistry departments who adhere to objective guidelines that are revised periodically. These include a description of lecture and laboratory content at various stages of instruction, the availability of certain scientific instruments and reference books and chemical journals the library needs to have. The objective is for students to receive a broad and comprehensive chemical education. An exchange of ideas about this topic for crystallography was addressed recently by Katharine Kantardjieff (**doc.fullerton.edu/~kkant/**), member of the ACA Committee on Education and Chair of the USNCCr Education Subcommittee; she organized an Education Summit in June 2005 which will result in a Policy Statement for crystallographic education at all age levels.

So, how are scientists perceived? Do people trust and respect scientists? While the widespread expressions "mad scientist", "geek" and "nerd" may seem like benign descriptions for scientists, they mask an underlying distrust, and fear of science. These feelings might result from transference of fear and anxiety over events such as environmental disasters, war, and terrorism. Scientific progress is sometimes equated with an increase in certain health, environmental and societal problems. Ignorance exists regarding the great strides that science has made in our lives, among the general population.

Frequently encountered attitudes are: (1) that science is not relevant; that people can exist very well without "complex" clarification and may argue that having a scientific explanation takes away part of the romance associated with living; (2) that science is too difficult - one must be a genius to become a member of the scientific community; (3) more antagonistic views regard scientists as dense, obtuse beings fixated on their beliefs. The lack of trust or understanding in science leads to a belief in non-rational explanations.

How do we stop this decline in scientific literacy? Today's young students will become tomorrow's consumers, leaders and lawmakers. They need to become scientifically literate so they can lead productive lives and have the knowledge to make essential decisions on scientifically based topics. Among other things, they need to know: that the scientific method can be used to make rational decisions; how to interpret data correctly; and how to recognize the limitations of the data. While we wait for more formal policies to take place, particularly our K-12 teachers need to know that they can count on us, the specialists, to augment what is on local curricula, by volunteering to visit schools, performing age-appropriate experiments, and arranging school field trips to scientific institutions. Internships for students to work in a laboratory can be set up even at an early age.

Those that can *should* rebut anti-science rhetoric whenever it is encountered. Examples are letters to the editor, and short general talks given for neighborhood associations. (A case in point is the monthly series *Science Without Fiction* that Josh Bloom, a pharmaceutical chemist wrote for the *Nyack Villager*, Nyack NY.) In short, we need to provide reminders for people that successful societies have always been technologically and scientifically superior to those around them and that, consequently, supporting and respecting science and scientists is essential to achieve this objective.

Miriam Rossi

Science Fiction Movie Mystery

Dear Judy, I've come across a minor pop culture mystery that I might enlist your readers to solve. As a Christmas present this year, I received a DVD of George Lucas' first feature film, a science fiction movie titled "THX 1138" (filmed in 1969-1970). While watching it, I suddenly noticed a brief shot of an x-ray diffractometer! The movie has nothing to do with crystallography or with science, for that matter, so somebody must have just gotten a shot of a "cool looking" machine and put it in the movie. I wonder if we could find out to whom this instrument belonged and how it happened to get into Lucas' film?

I've attached a JPEG of a screen capture of the diffractometer in the movie. In order to see a clip of the scene in which this appears, go to my website: **macxray.chem.upenn.edu** (bottom of first page). Actually later in the scene there is also a shot of a precession camera.

Patrick J. Carroll, U. Pennsylvania

Intelligent Design in the UK

Dear Connie, Thank you for raising the issue of Intelligent Design (= Creationism) and its fundamental dangers to the US education system. This issue has also reared its head in the UK in recent years, as noted in the *Guardian* article by Dawkins & Coyne that you cited. In the USA you have a secular education system and there has also been open national debate, together with determinations through judicial processes (as in the recent Dover, PA ruling). The UK situation is more complex, and the creationist issue has crept in via the back door of government policy on the organization and funding of schools. Some very brief background is necessary.

In the UK, the mainstream churches, particularly the established Anglican church, played a significant historical role in developing the educational system. Various acts of Parliament from the late 1800s, and particularly the 1944 Education Act, fully integrated church schools within a state system and enshrined the concept of daily worship in all state schools, a requirement that was reiterated in 1988. Roman Catholic, Moslem and other faith-based schools are also an integral part of state educational provision. Nevertheless, within this non-secular system, science has firmly remained science, and religious education has remained religious education. However, in a few schools there is now a crossing of these boundaries.

Recently, the UK government has become very keen on developing the education system in partnership with private organizations. Here, faith-based organizations, business enterprises, etc. contribute funds towards the establishment of a school and in return play a significant role in how the school is organized and operated. While this policy is promoted as 'diversifying' the system and encouraging new funding, it also opens a back door for organizations with strong ideological views to gain a foothold in the educational process. It is for Local Education Authorities or the government, under whose aegis these schools must operate, to determine if such views exist and are educationally appropriate, before any partnering can be agreed upon.

As part of this policy, the UK Government has encouraged the private-state partnership model to flourish in the establishment of new 'city academies', operating as largely autonomous units within the state system. One of these 'private' partners has been the Vardy Foundation. Sir Peter Vardy is a wealthy motor vehicle dealer in the north-east of England. His company currently sponsors Sunderland Football Club, and his Foundation does charitable works in the local area. Vardy, however, is a Christian fundamentalist, and the Foundation has contributed significant sums of money to the establishment of city academies, most notably Emmanuel College in Gateshead, and the King's Academy in Middlesborough. This has opened the door to the teaching of creationism alongside evolution in science lessons. This inappropriate activity has been well publicized by the British Humanist Association (BHA: **humanism.org.uk**), the news media (*e.g.* the *Guardian:* **guardian.co.uk**), and has prompted letters to the Prime Minister from concerned scientists as well as questions in Parliament. The interested reader should search the BHA and *Guardian* websites for 'creationism' to obtain a more complete summary of recent UK happenings, plus many links to the issue in both the UK and the USA.

One (officially documented) British parliamentary interchange cited by the BHA involved a Member's question (13 March 2002) on whether the Prime Minister was *"happy to allow the teaching of creationism alongside Darwin's theory of evolution in state schools."* Mr Blair replied that he ***was*** happy and that *"it would be unfortunate if concerns about that issue were seen to remove the very strong incentive to ensure we get as diverse a school system as we properly can…"* This is truly scary rhetoric, and taken to its extreme it generates a worrying definition of 'education': so long as you are rich enough, you can buy the power to manipulate young minds.

However, the publicity is now having an effect. In late 2005, and despite central government pressure, a campaign by concerned parents in Yorkshire persuaded their Local Education Authority to reject a Vardy Foundation bid to sponsor a city academy in Doncaster. Furthermore, Professor Lord May, speaking as outgoing President of the Royal Society of London, also raised the creationism issue very strongly. He exhorted scientists to be more proactive in making their voices heard: *'The scientific community should be energetically engaging the political process in all avenues that can be pursued."* (*Guardian,* 30 November 2005.)

Scientists in both of our countries would do well to heed these words, and I congratulate you on raising the issue in the *ACA Newsletter*.

Frank Allen, Cambridge, UK.

ID News Update from the Editors:

In *Science's* "Breakthrough of the Year" issue December 23rd, the editors put at the top of their list of top 10 research advances for 2005 the new insights about evolution at the genetic level and the birth of the species. The accompanying news story (p. 1878) described the reasons that "2005 stands out as a banner year for uncovering the intricacies of how evolution actually proceeds." For an expanded version of the article see **sciencemag.org/sciext/btoy2005**. The AAAS also has an informative "Evolution on the Front Line" website: **aaas.org/news/press_room/evolution/.** One of the items to be found there is the AAAS board resolution on intelligent design, a clear, concise and compelling statement.

Meanwhile, -- from the National Center for Science Education website: **ncseweb.org**, (except where otherwise noted), --in the real world that includes lots of non-scientists:

Utah: From the *Salt Lake Tribune*, Jan 30, 2006: Utah's **Senate Bill 96** was passed by the Senate on January 23, 2006, by a 16-12 vote. If enacted, **SB 96** would direct the Utah state board of education to require "that if instruction is given to students on any theory regarding the origins of life, or the origins or present state of the human race, then that instruction shall stress that not all scientists agree on which theory is correct" and to "ensure that all policies and positions of the State Board of Education relating to theories regarding the origins of life or the origins or present state of the human race: (i) do not endorse a particular theory; and (ii) stress that not all scientists agree on which scientific theory is correct." The bill was subsequently introduced in the State House of Representatives on January 24, and is expected to win approval.

AAAS CEO Alan I. Leshner, writing in the January 29 *Salt Lake Tribune* had warned that this measure targeting evolution education would pose a risk to upcoming generations of science, technology and medical researchers. He said it "would encourage students to doubt the science of evolution and perpetuate the myth that evolution is challenged by 'opposing scientific viewpoints'."

Mississippi: **House Bill 953** and **Senate Bill 2427** were introduced and referred to their respective Committees on Education in January, 2005. Previous bills with similar language have died in committee; however, if enacted, **HB953** would enable Mississippi school boards "to authorize the teaching of 'creationism' or 'intelligent design' in the public schools." Moreover, "if the school's curriculum requires the teaching of evolution, then the teaching of 'creationism' or 'intelligent design' shall be required." **SB2427**, if enacted, would ensure that "no local school board, school superintendent or school principal shall prohibit a public school classroom teacher from discussing and answering questions from individual students on the issue of flaws or problems which may exist in Charles Darwin's Theory of Evolution and the existence of other theories of evolution, including, but not limited to, the Intelligent Design explanation of the origin of life."

Then, in January, 2006, antievolution bills were introduced in **Oklahoma** (**HB2107, HB2526, SB1959**); in **Alabama** (**HB106**, **SB45**); in **Indiana** (**HB1388**); in **Missouri** (**HB1266**) and in **Michigan** (**HB5606**).

Kansas: We can't resist adding to our winter issue update the news (via a note in *Science* Dec. 2nd) that the card game BONE WARS: *The Game of Ruthless Paleontology*, available online from **zygotegames.com** offered a special 20% discount through January, 2006 to anyone buying from or shipping to Kansas. When the Kansas Board of Education failed in their attempt to give equal status to the teaching of Intelligent Design, and so tried instead to redefine science to include the supernatural - Zygote Games thought they obviously had a lot to learn in Kansas about how a scientific theory is developed and tested.

Pennsylvania: On December 20th, Judge John Jones III ordered the Dover, PA schools to remove references to Intelligent Design from the science curriculum.

Parents had sued after the Dover school board passed a resolution in October, 2004 declaring that "students will be made aware of gaps and problems in Darwin's theory and of other theories of evolution including, but not limited to, Intelligent Design." (As reported in our winter update column, eight members of that school board were replaced last November by new members staunchly unsympathetic to ID.) Excerpts from Judge Jones' decision (*Science*, Jan. 6, 2006): 1) ID violates the centuries-old ground rules of science by invoking and permitting supernatural causation; 2) The argument of irreducible complexity, central to ID, employs the same flawed and illogical contrived dualism that doomed creation science in the 1980s, and 3) ID's negative attacks on evolution have been refuted by the scientific community . . . It has not generated peer-reviewed publications, nor has it been the subject of testing and research. . . .

Such irresistibly lucid arguments. However, it happened that when this welcome news broke, one of us (Connie) happened to be in Shamrock, TX, where bad weather and black ice had forced an overnight stay. The evening was spent discovering that not only did her cell phone not work, but out of umpteen cable channels on TV, the only network news available was Fox -no CBS, NBC, or ABC. The next morning a vain attempt to find an NPR station was made on the car radio, but the only newscaster-sounding voice was bemoaning the fact that an extremely biased, unreasonable judge had the audacity to rule that they couldn't teach children in Pennsylvania the simple facts that most people believe in! What a travesty of justice!

Art in Crystallography Prize

The Editors are currently accepting entries for the ***Art in Crystallography Prize,*** sponsored by the *ACA Newsletter* and the ACA Council. Entries should be sent in the form of images emailed to either of the Editors (**conniechidester@earthlink.net** or **flippen@rcsb.rutgers.edu**). Each entry should be accompanied by a paragraph explaining the science and the method of producing the image. A photo of the artist would be appreciated but is not required. Prizes will consist of a small monetary award plus a banquet ticket and waiver of registration fees at the annual meeting. Please see the fall or winter 2004 *ACA Newsletters* for more details, or ask the Editors via email.

Suzanne Fortier Appointed President of NSERC

On November 23, 2005 The Hon. David L. Emerson, Minister of Industry and Minister responsible for the Natural Sciences and Engineering Research Council of Canada (NSERC), appointed **Suzanne Fortier** as President of NSERC. He said "With her leadership, experience and expertise, I am pleased to welcome Dr. Fortier as President of NSERC; I am confident that her contributions will enable Canada to remain at the forefront of growth and advancement in university research and researcher training."

On January 16, 2006, Suzanne officially started her duty as the fifth President of the Council. She said "I have long recognized the important role NSERC plays in supporting research and innovation, and I look forward to working with the Council's many stakeholders across Canada." She had been a member of NSERC's Council from 1996 until July 2005, and served a term during this period as Vice-President of the Council.

NSERC is an offshoot of the NRC of Canada. Through NSERC Scholarships and Fellowships and NSERC Discovery Grants, the agency supports some 22,000 university students and postdoctoral fellows; funds more than 10,000 university professors every year; and fosters innovation by encouraging more than 600 Canadian companies to participate and invest in university research projects.

Suzanne obtained her undergraduate degree and her Ph.D. from McGill University. After holding research positions at the Medical Foundation of Buffalo and the National Research Council of Canada, she joined the faculty of Queen's University in 1982. She went on to become a full professor in both the Chemistry Department, and Computing and Information Science. Her research was concerned with the development of mathematical and artificial intelligence methodologies for protein structure determination and crystallographic data mining. She co-directed (with Janice Glasgow) the Molecular Scene Analysis Laboratory at Queen's. Suzanne was appointed Vice-Principal (Academic) at Queen's from 2000 to 2005. In addition, she was on the Board of Directors for the Ontario Centres of Excellence, Inc., chaired the Ontario Science and Innovation Council (OSIC), and is a member of the Board of Governors for the Royal Military College of Canada. She has received numerous awards, including a Distinguished Service Award from the Queen's University Council for her exceptional contributions to research and academics and her devotion to Queen's University. In 1997, Suzanne directed the very successful and memorable 25th Summer Course in Erice, Italy: *Direct Methods of Solving Macromolecular Structure*.

Photo courtesy of J.A.Lippard

http://web.mit.edu/chemistry/lippardlab/

Stephen Lippard Awarded National Medal of Science

Stephen J. Lippard, the Arthur Amos Noyes Professor of Chemistry at MIT, was awarded the 2004 National Medal of Science by President George Bush November 14, 2005.

The award, established by Congress in 1959, honors individuals "for pioneering scientific research in a range of fields, including physical, biological, mathematical, social, behavioral, and engineering sciences, that enhances our understanding of the world and leads to innovations and technologies that give the United States its global economic edge."

Stephen was cited "for pioneering research in bioinorganic chemistry, including the interaction of metal compounds with DNA, preparation of synthetic models for metalloproteins, and structural and mechanistic studies of methane monooxygenase."

He responded "I am very pleased to receive this honor for it recognizes the work of the many wonderful graduate students and post-doctoral associates who have contributed to the science that we were able to accomplish; it was most unexpected."

Stephen's current research includes structural and mechanistic studies of platinum anti-cancer drugs, the synthesis of dimetallic complexes as models for non-heme iron enzymes and metallohydrolases, mechanistic studies of methane monooxygenase, and the development of reagents for studying neurochemical signaling, especially fluorescent probes for zinc and nitric oxide. He obtained his undergraduate degree from Haverford College and his PhD from MIT. He joined the faculty at Columbia University in 1966, and was promoted to full Professor in 1972. He returned to MIT in 1983, and headed the Chemistry Department 1995-2005. He has received numerous awards and prizes, has authored or co-authored more than 640 articles, holds several U.S. and foreign patents, and has written or edited two textbooks. His book with Jeremy Berg is *Principles of Bioinorganic Chemistry*. Among his many activities he is an Associate Editor of *JACS*, is an ACA member, and is an avid harpsichordist, early morning jogger, and occasional horseback rider.

Draper Prize to CCD inventors

The National Academy of Engineering announced that physicists **George Smith**, 75 and **Willard Boyle,** 81, will share the $500,000 **Charles Stark Draper Prize** (2006) "for the invention of the Charge-Coupled Device (CCD), a light-sensitive component at the heart of digital cameras and other widely used imaging technologies." Their discovery was made in 1969, at Bell Labs.

Willard Boyle (left) and George Smith (right) demonstrating a TV camera that uses a CCD.

Photo courtesy of Lucent Technologies Bell Labs.

World Technology Award to Nadrian Seeman

Nadrian Seeman, Professor of Chemistry, New York University, was recently awarded the 2005 **World Technology Award for Biotechnology** by the World Technology Network. Seeman and his research team at NYU have focused their efforts on exploiting the natural tendency of branched DNA to assemble itself into coherent structures. Due to intermolecular forces, unpaired DNA strands seek out and "stick" to complementary strands. As a result, biological systems are able to self-assemble their components into complex molecular structures on the nanometer scale. One of their devices allows for the translation of DNA sequences, thereby serving as a factory for assembling the building blocks of new materials. This device, developed with NYU Chemistry graduate student Shiping Liao, emulates the process by which RNA replicas of DNA sequences are translated to create protein sequences.

New Website; Crystal Answers: A new forum for the discussion of x-ray crystallographic topics is available on the web at **crystalanswers.net/phpbb.** **Crystal Answers** was developed to provide a place for the public exchange of ideas, advice, tips and problems relating to all aspects of crystallography. All are welcome to join and participate in this independent, non-sponsored forum. Registration is free. If you have crystal questions, check out **Crystal Answers**!

Amy Sarjeant, Johns Hopkins University

note: a link to Crystal Answers is now on the ACA website.

ACS Award to Raquel L. Lieberman

The **ACS 2006 Nobel Laureate Signature Award for Graduate Education in Chemistry** (sponsored by Mallinckrodt Baker Inc) will be presented to **Raquel L. Lieberman** on March 29th in conjunction with the ACS annual meeting in St. Louis. **Amy C. Rosenzweig**, Northwestern Univ. will be recognized as her preceptor. (Amy did her Ph.D research in Stephan Lippard's lab at M.I.T., and although they did not overlap there, Raquel also worked in Stephan's lab as an undergraduate.)

Raquel was recognized for solving the first crystal structure of particulate methane monooxygenase, an integral membrane metalloenzyme that catalyzes the oxidation of methane, the most inert hydrocarbon, to methanol, an important contribution to the understanding of membrane proteins.

Currently, Raquel has an NIH-NRSA Postdoctoral Research Fellowship at Brigham & Women's Hospital / Harvard Medical School and Brandeis University, and is studying proteins implicated in Alzheimer's disease.

75th Anniversary of the AIP

The American Institute of Physics (AIP) is celebrating its 75th anniversary during 2006. AIP's keynote event will take place May 3-5, 2006, with a two-day series of talks, receptions, exhibits, and the semi-annual meeting of its Governing Board. Highlights include talks by Presidential Science Adviser John Marburger, Nobel Laureate Steven Chu, and National Academy of Sciences President Ralph Cicerone. Throughout the year, AIP's *Journal of Applied Physics (JAP)* will be holding a concurrent celebration of its 75th anniversary.

New Name for Newsletter; Logo Possibilities

Inspired by the news magazine published by the mineralogy community (8 organizations) called ***Elements*** (**elementsmagazine.org**), the ACA Council and the Editors decided that we needed a new name for our news "magazine." Council suggested ***Reflections***; and the Editors liked that name, so we are trying it out with this issue. Please let us know if you like it or not.

We also think it is time that we updated our ACA logo. These days not so many of us have ever used or even seen a Weissenberg camera. In this issue and following issues we will try out some possibilities in the header lines. The samples in this issue were designed by Vanessa Vair.

2006 Appropriations, a Disappointing Year for R&D Funding

On December 30, nearly three months into the fiscal year, President Bush signed the last two FY 2006 appropriations bills into law, bringing the FY 2006 appropriations process to a close. AAAS estimates that the federal R&D portfolio totals $134.8 billion in 2006, a $2.2 billion or 1.7% increase. But 97% of the increase goes to just two areas: defense weapons development and human space exploration technologies. Funding for all other federal R&D programs collectively will barely increase, and will fall nearly 2% after adjusting for inflation. Leaving out large federal investments in development, congressional appropriations for basic and applied research total $57 billion, an increase of $1 billion or 1.8% over 2005. But NASA applied research on human space flight technologies accounts for a majority of the increase, leaving most agency research portfolios with modest increases falling short of inflation, or cuts.

Many flagship federal science agencies have disappointing budgets in 2006: the National Institutes of Health (NIH) budget falls for the first time in 36 years; the National Science Foundation (NSF) wins a small increase but has less in real terms for its research portfolio than in any of the last three years; the Department of Energy (DOE) Office of Science budget declines, and despite big increases in development funding, the Department of Defense (DOD) basic research funding declines.

Call for Nominations for Margaret Etter Early Career Award, 2007

The Margaret C. Etter Early Career Award recognizes outstanding achievement and exceptional potential in crystallographic research demonstrated by a scientist at an early stage of their independent career. The recipient will receive a monetary award and a plaque and will present a lecture at the 2007 ACA Meeting. Please see the winter 2004 *ACA Newsletter* (p64) for details about the award and about Margaret Etter.

Scientists involved in crystallographic research in the broadest sense will be eligible for the award. Nominees must have begun their first independent (not postdoctoral) position within the past 6 years (not including career breaks). Nominations, (send to **marcia@hwi.buffalo.edu**), must include a nomination letter clearly indicating accomplishments since the nominee began an independent career and assessing future potential. Additional supporting letters and a *c.v.* may be provided but are not required. Self-nominations are not permitted. Nominees may be employed in academia (including service crystallography), in industry or in government laboratories. **The deadline is September 1st, 2006,** but please send nominations as soon as possible.

The ACA Summer Course in Small Molecule Crystallography, 2006

This course will be offered July 10th through July 19th, 2006 at the Indiana University of Pennsylvania, in the town of Indiana, PA located about 80 miles east of Pittsburgh. Each day there will be three lectures in the morning on single crystal and powder diffraction methods, followed by various workshops and computer tutorials. These will cover a wide range of topics including Reitveld analysis, problem solving, data analysis and crystal structure determination. The curriculum will emphasize the underlying scientific principles of x-ray crystallography. Attendees are expected to have completed at least undergraduate courses in chemistry, physics and mathematics. In the past, we have had successful attendees from biology, chemistry, geoscience, physics and materials science. No prior experience of x-ray crystallography will be assumed, but attendees are advised to read in advance "*Crystal Structure Analysis: A Primer*", by Jenny P. Glusker and Kenneth N. Trueblood, Oxford Univ. Press (1985).

The organizers aim for a total of 25 attendees, who in past years have come from academia (students and faculty), government and corporate institutions, both in the U.S. and from abroad. There will be at least 12 experienced teaching faculty. Tuition and board will be $650 ($1000 for applicants from corporate labs). This covers tuition, single student apartment housing at IUP, breakfast and lunch). Up to 12 graduate student scholarships will be offered. These will consist of a waiver of tuition and living costs (double occupancy). The scholarships will be awarded based on the student's (1) scientific ability, (2) expected benefits from the course and (3) skills in English. We encourage applications from Latin America.

The instruments available on site will be three Bruker-Nonius diffractometers (a CAD4 and D8 Advance at IUP and an APEX instrument with CCD detector located at the University of Pittsburgh and electronically linked to the Lab at IUP). In previous years, Rigaku and Bruker have set-up state-of-the-art instrumentation for use in the course including a Rigaku Miniflex powder diffractometer, Rigaku SPIDER single crystal instrument and a Bruker APEX II single crystal instrument. The computer labs will have ample space and each attendee will have access to an individual computer. The facilities will include access to the Cambridge structural data base and the ICDD PDF-4 powder diffraction data base.

The Course registration form can be obtained from the ACA web site at **hwi.buffalo.edu/ACA/**. Completed forms must be received before June 2nd, 2006 by Bryan Craven, Chemistry Department, Indiana University of Pennsylvania, Indiana, PA 15705, USA or electronically by Charles Lake. Further information will be updated on the web site or can be obtained from **Lake@iup.edu** or **craven@icubed.com.**

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

Bryan M. Craven and Charles H. Lake, Organizers.

ACA Council News: Highlights of Fall 2005 Council Meeting

The ACA Council met on Sunday, November 6th, in Arlington, VA. *ACA Newsletter* Co-Editor, Judy Flippen-Anderson attended to discuss the evolution of the *Newsletter*. **Note the new name on the cover.** Over the years, the *ACA Newsletter* has transformed dramatically, from the black and white print and photos to the glossy and colorful publication of today. The *Newsletter* has expanded in size and content and is valued as a significant forum for communication within the community. All crystallographers are invited to contribute news items and comments.

ACA Business: This was the last Council meeting for which Louis Delbaere served as President. In his report to Council, he reviewed the events of the last year, highlighting significant milestones. A new category of membership, the Latin-American Country Membership, was formed and Argentina and Brazil were accepted as members. The May 2005 annual meeting in Orlando, FL was very successful, and featured outstanding scientific presentations. Delbaere thanked the members of ACA council and the staff at ACA headquarters. Since this was the last council meeting for Frances Jurnak, who concluded her term as Past President, best wishes and gratitude were expressed. Robert Bau now steps up to the Presidency, and will lead the ACA for the year 2006.

The July 2006 Meeting in Hawaii: The 2006 Annual ACA Meeting is scheduled for July 22 - 27 at the Sheraton Waikiki Beach Hotel in Honolulu, Hawaii. There will be a half day session entitled *International Macromolecular Crystallographic Advances* on the first day of the meeting. This promises to be a very exciting session, with speakers from the Pacific Rim countries, and offers a unique opportunity for scientific exchange across international boundaries. The **Buerger Award** will be presented to **Helen Berman** in recognition for her development of information services, including the Protein Data Bank (PDB), the Nucleic Acids Database, and the Research Collaboratory for Structural Bioinformatics (RCSB). The **Warren Award** will be presented to **Charles Majkrzak** for his contributions to the development of neutron reflectivity and its use in interface science. The **Etter Early Career Award** will be presented to **Carrie Wilmot** for her work on post-translational modifications of proteins. The meeting commences with workshops on: neutron protein crystallography; management of synchrotron image data; and grazing incidence SAS with x-rays and neutrons. The *Transactions* Symposium will be on neutron diffraction of small molecules and macromolecules. **The early registration deadline for the ACA 2006 meeting is June 1, and since the penalty for late registration is significant, early registration is strongly encouraged.**

Future Meetings: Sites for the next two annual meetings have been determined. The 2007 meeting will be in Salt Lake City, UT and the 2008 meeting will be in Knoxville, TN.

Lisa Keefe

Please note: VISA Alert

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

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

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Web Watch:

Members of the Communications Committee of the ACA encourage everyone to participate in the Crystallography Web Watch Column. The web address of web sites of interest to crystallographers and a brief description should be sent to Louis Delbaere at louis.delbaere@usask.ca. Thank you in advance for any suggestions.

Crystallography:

(IUCr) Crystallographic CourseWare: to assist people in learning crystallography: **scripts.iucr.org/cgi-bin/paper?os0010**

Crystallography education Websites: hwi.buffalo.edu/ACA/CrystalEducationSites.html

Tutorial on symmetry and space groups: people.brandeis.edu/~foxman1/teaching/indexpr.html

Biological Sciences:

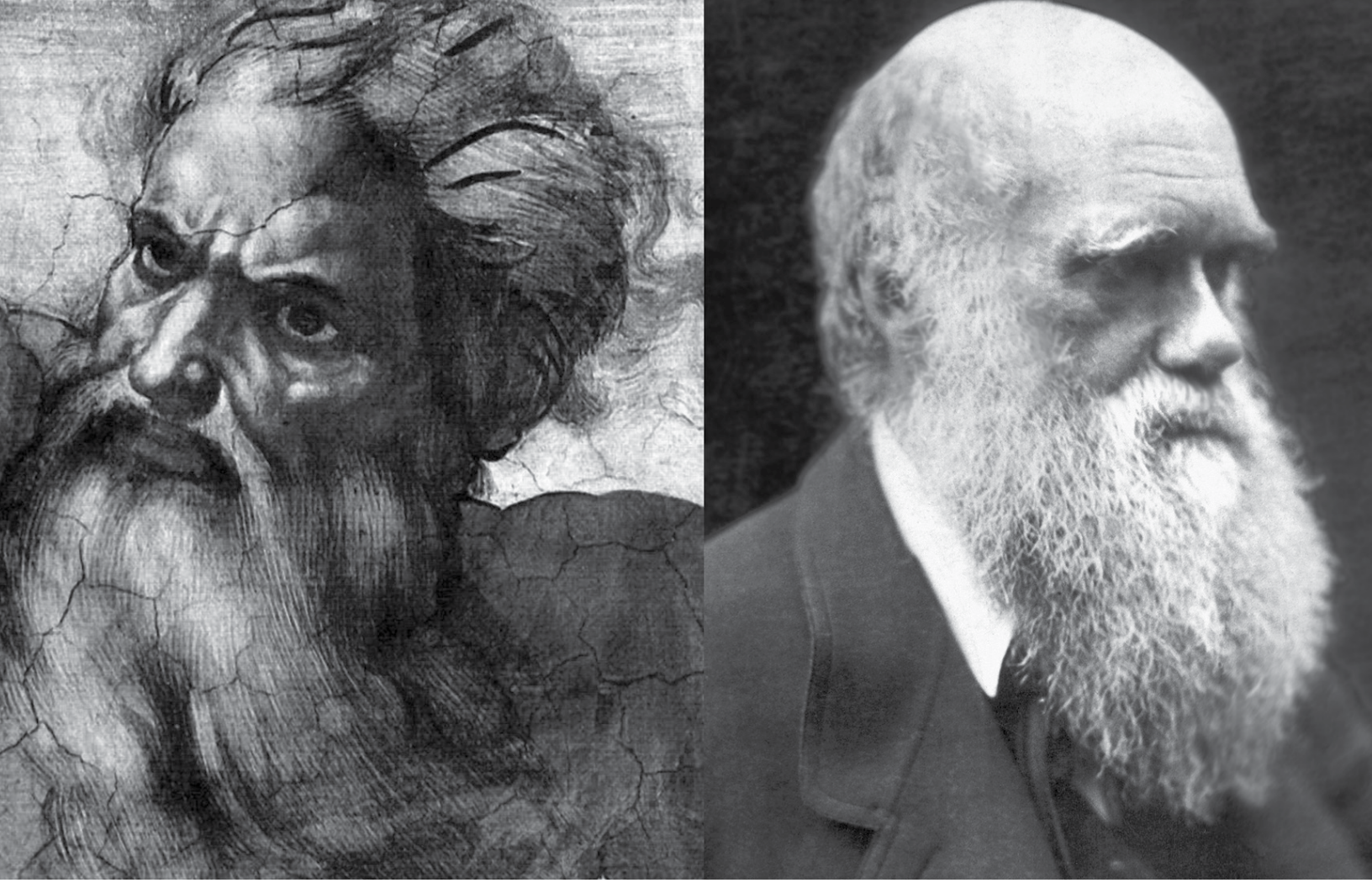
BEN (BiosciEdNet) is a digital library for teaching in the biological sciences, managed by AAAS; there are 4,100 reviewed resources and registration is free: **biosciednet.org/portal/**

BioResearch is a free catalogue of hand-selected and evaluated Internet resources, covering the biological and biomedical sciences: **bioresearch.ac.uk/**

Online biological references and journals: science.gov/browse/w_115.htm

New discoveries for the technically minded:

Slashdot is very good for the technically minded person; it picked up the PNAS reference on BioGlas, which induces proteins to crystallize and may revolutionize protein crystallization: **slashdot.org/**



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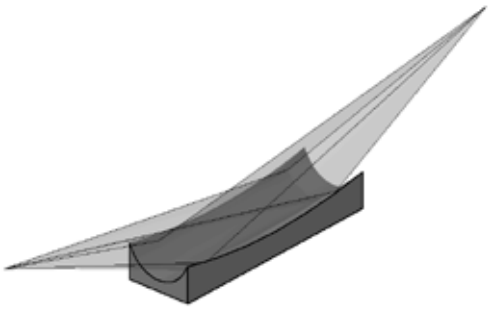

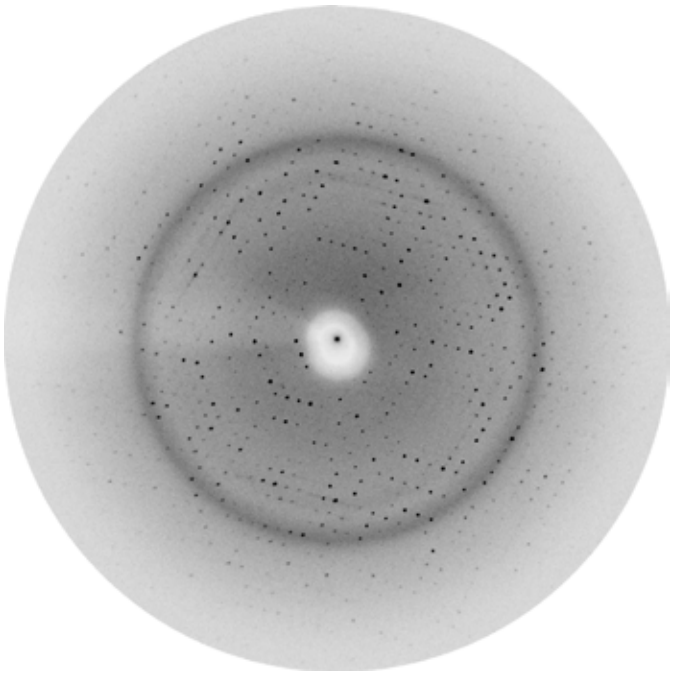

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Data Courtesy of Dr. Andrew GW Leslie
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The crystal belongs to space group C222 with cell dimensions a=72.1Å, b=97.4Å, c=191.0Å. Images were collected with an oscillation angle of 0.4˚.
The crystal was a thin plate with approximate dimensions 200x75x50 µm³.
The generator was a Rigaku RuH3R running at 50kV, 100mA (300 µm focus) and the data were collected on a Mar345 image plate detector.

	classical confocal multilayer system	Xenocs *FOX2D CU 25_25P*
Exposure time per frame	4 min	4 min
R_{merge} (22.7.-2.43A)	8.8%	6.4%
R_{merge} (2.57-2.43A)	44.1%	26.2%
<I>/<sigI> (22.7.-2.43A)	12.1	15
<I>/<sigI> (2.57-2.43A)	2.5	4.1
Mean multiplicity	3.3	3.3

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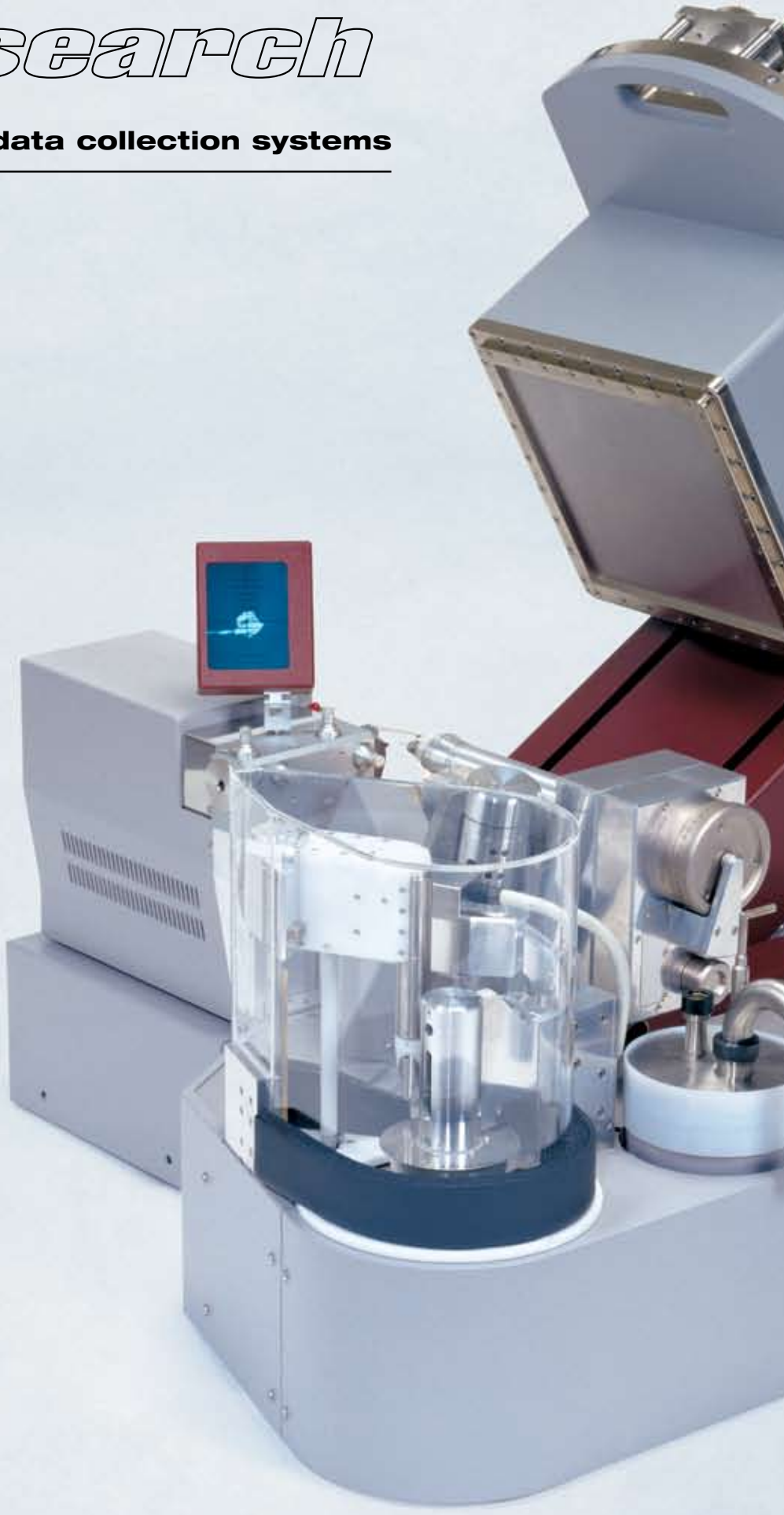

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Robinson D. Burbank (1921 – 2006)

Rob Burbank during his tenure at Bell Labs

Robinson Derry Burbank, President of the American Crystallographic Association in 1975 and Bell Labs scientist who worked on the Manhattan Project, died February 9, 2006 at his home in Summit, NJ following a brief illness.

Rob was born October 3, 1921 in Berlin, NH, graduated *Phi Beta Kappa* from Colby College in 1942 and received his PhD in inorganic chemistry from MIT in 1950. He performed spectrochemical analysis on uranium and thorium at MIT during World War II as part of the Manhattan Project. Upon completing his doctorate, he joined the Gaseous Diffusion Plant in Oak Ridge, Tennessee as a senior physicist before coming to Bell Laboratories in Murray Hill, NJ in 1955. His contributions to greater accuracy in structural investigations included his early demonstration of the value of cooling the crystal under investigation to low temperatures, his recognition of the geometric conditions under which intrinsic multiple diffraction occurs and his comparisons of the use of ω and 2θ scans for integrated intensity measurements. Materials of unusual chemistry and physical properties, including noble gas and interhalogen compounds such as $XeF_2 \cdot IF_5$ and XeF_6, the structures of which he detetermined, were also among his interests as were the mechanisms of phase transitions. He published more than 50 articles in scientific journals.

He was a charter member of the ACA, and in addition to serving as President in 1975, was ACA Treasurer from 1965 - 1968. He was a member of the American Physical Society and of the American Association for the Advancement of Science. He served on the executive committee of the Governing Board of the American Institute of Physics and was a U.S. delegate to the International Union of Crystallography in 1975.

A ski-jumper in his youth, Rob Burbank was an avid skier, hiker, and mountain climber. He was a longtime patron of the arts, especially the Metropolitan Opera. He is survived by a son, Paul R. Burbank of Ozone Park, NY, a daughter, Claudia Burbank of Bernardsville, NJ, and two granddaughters, Christine and Joy Burbank of Kew Gardens, NY. Contributions in his memory may be made to the Mount Washington Observatory, P.O. Box 2310, North Conway, NH 03860, or to the Metropolitan Opera Company in New York.

Reuben Rudman (1937-2006)

The unexpected word of Reuben Rudman's death on February 16, 2006 came as a shock to his many friends and colleagues. He died in Israel where he had just finished teaching a graduate course on structural chemistry at the Hebrew University in Jerusalem and was planning to return to the US next week. Reuben was a long time, active member of the ACA; a full obituary will be published in a later issue of the *Newsletter.*

Sidney Abrahams

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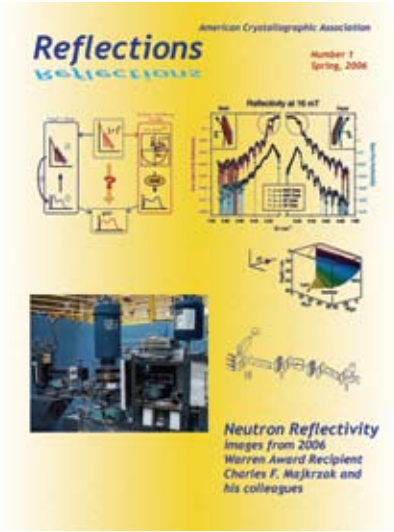
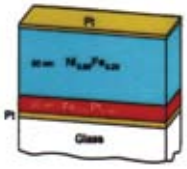
Images from Charles F. Majkrazk, 2006 Warren Award Recipient and his Colleagues



At lower left is a photograph, corresponding to the diagram at lower right, of the polarized neutron reflectometer / diffractometer located on the NG-1 guide tube at the NIST Center for Neutron Research (NCNR) in Gaithersburg, Maryland. This instrument is used to study the nano- and atomic-scale magnetic structures of thin films and superlattices. With polarized neutrons, both the magnitude and direction of the vector magnetization depth profile can be obtained with subnanometer resolution along the normal to the surface.

The schematic at lower right illustrates the essential components of a polarized neutron reflectometer / diffractometer. Cold neutrons, with wavelengths of the order of 5 Å, which emanate from a liquid hydrogen cold source are transported through a guide to a monochromator that selects out a narrow wavelength band (of the order of 1%) and simultaneously focuses the beam along the vertical direction. Pairs of slits, up- and down-stream of the sample, limit the angular divergence in the scattering plane defined by incident and reflected wavevectors. In addition, Fe/Si thin-film multilayer devices or "supermirrors" polarize the incident beam and analyze the polarization state of reflected neutrons (in transmission). Rectangular magnetic field coils enable the polarization state of the neutron to be rotated relative to a defined magnetic field direction or axis of quantization. "Neutron scattering studies of magnetic thin films and multilayers," C.F.Majkrzak, *Physica B* **221,** 342-356 (1996); "Advances in polarized neutron reflectometry," C.F.Majkrzak, *Physica B* **213** & **214**, 904-909 (1995); "Magnetic Rare-Earth Superlattices," C.F.Majkrzak, J.Kwo, M.Hong, Y.Yafet, D.Gibbs, C.L.Chien and J.Bohr, *Advances in Physics* **40**, 99 (1991).

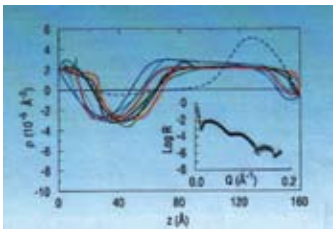
Accompanying these, the image at upper right shows polarized neutron reflectivity data, top, which reveals the vector magnetization depth profile (below) of the magnetic thin film sandwich structure.



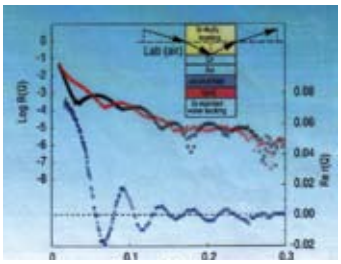
A schematic of the thin film sandwich structure deposited using magnetron sputtering. The magnetic films are FePt and NiFe alloys.

"Pinpointing Chiral Structures with Front-Back Polarized Neutron Reflectometry," K.V.O'Donovan, J.A.Borchers, C.F.Majkrzak, O.Hellwig, and E.E.Fullerton, *Physical Review Letters* **88**, 67201 (2002).

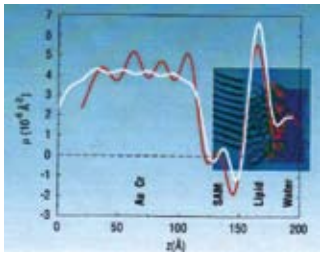
The image at upper left is a flow diagram for the analysis of specular neutron reflectivity data in the dynamical regime. On the left is shown the conventional analysis which essentially involves fitting by sophisticated trial and error. Indicated on the right is the first-principles method for exactly determining the reflection amplitude, uniquely at each wavevector transfer. (This can be accomplished through the use of reference layers or substrates adjacent to a common "unknown" film of interest.) The corresponding scattering length density depth profile, along the surface normal, can then be obtained by direct inversion of the reflection amplitude using the Gel'fand-Levitan-Marchenko (GLM) integral solution. "Exact determination of the phase in neutron reflectometry," C.F.Majkrzak and N.F.Berk, *Physical Review B* **52,** 10827 (1995); "Exact determination of the phase in neutron reflectometry by variation of the surrounding media," C.F.Majkrzak and N.F.Berk, *Physical Review B* **58,** 15416 (1998).



To help explain the flow diagram, the figure at left illustrates the ambiguity that can result in the scattering length density profile extracted from a single set of reflectivity data (insert at lower right). The film structure is that of TiO on Ti. The family of solid curves for the scattering length densiy profile generate a fit to the measured reflectivity data that is as good as that obtained for the dashed curve!



The figure at right shows two neutron reflectivity data sets (black and red symbols) collected for the same Cr / Au / alkane thiol / lipid film structure (schematically represented in the inset) but deposited on two different substrates, one silicon, the other sapphire. From the two composite reflectivity data sets, the real and imaginary parts of the reflection amplitude corresponding to the "unknown" film of interest alone, in this case consisting of the Cr / Au / alkane thiol / lipid layers, can be solved for uniquely and independently at each wavevector transfer.



At left, a comparison of the results of a direct inversion of the reflection amplitude above using the GLM integral solution (red curve). This is compared to a molecular dynamics simulation for the alkane thiol and lipid layers on the gold beneath (white curve). The unphysical ripples in the Au / Cr region, which has a uniform, flat scattering length density, are an artifact of the truncation of the measured reflectivity at a maximum wavevector transfer (~ 0.3 inverse Å). "First-Principles Determination of Hybrid Bilayer Membrane Structure by Phase-Sensitive Neutron Reflectometry," C.F.Majkrzak, N.F.Berk, S.Krueger, J.A.Dura, M.Tarek, D.Tobias, V.Silin, C.W.Meuse, J.Woodward, & A.L.Plant, *Biophysical Journal* **79,** 3330-3340 (2000).

Patterson Award Address on Macromolecular Model Building and Validation – as recalled by Alwyn Jones

I was born in the front parlour of a small house in a small village in South Wales. Dad was a coal-miner and Mam looked after us. Our valley was U-shaped, mostly green, with black blotches. As a little kid I was always sick and Mam always packed me into as many layers as she could manage. I didn't speak much, except to an old man who sold things door-to-door from a suitcase who claimed to understand what little I did say. At the same time, the girls at the COOP used to put me on the counter and teach me poems, naughty poems. They thought it was hilarious, with me all wrapped up, seriously repeating what they'd taught in my funny little voice. I realize now that it was a good introduction to public speaking, if that's really needed for a Welsh man. When I was about six years old, Dad took me to the pit to show me the cage that took him underground every day. "Do you want to work down there?" he said."No", I replied. "Then you'd better study." he replied. I really didn't need such advice since I already liked school, and liked it even more as I got older.

By the time of my first day at grammar school, I had learned to talk, sort of. Indeed I got the first detention mark of the year's intake for not shutting up within about 5 minutes. The "offending" teacher taught mathematics (another Jones) and he became one of my favorites, He was one of many fine teachers, and indeed Pengam Grammar was a wonderful school despite forcing me to wear a tie and blazer. It produced a great rugby player in John Dawes (Captain of Wales, London Welsh, the Babas in the 1973 match against the All Blacks -Phil B to JPR to Dawes to Quinnel to Gareth, sorry), but failed to get get me to pronounce my "H's (another good introduction to public speaking "Henry held Henrietta's hand", repeated again and again and again for the amusement of my French teacher).

I left home in 1966 to study physics. Why physics? Because I was most interested in astronomy and I thought this was the best way of preparing myself. But it was not to be. At the end of my BSc, although it was still a close call, I ended up choosing structural biology. I didn't enjoy doing my doctorate but my interest in science perked up by attending the Alpbach conference that Max Perutz and Walter Hoppe organized in about 1972. It started off badly by my missing the plane because the clocks changed without telling me. I finally got to Munich railway station hours after the appointed time, and the only German I knew was limited, mostly gained from the comics I had read as a child. This was an opportunity to practice that well known game, "spot the crystallographer". Even when speaking a foreign language, crystallographers have a very distinctive body language. On the train to Innsbruck, I spotted a likely candidate who turned out to be Boris Vainshtein. Fortunately, the organizers had arranged a bus to pick him up and no one objected to my joining the group. I didn't know anyone at the meeting and nobody knew me so we were even. The conference, however, was spectacular and fired my resolve to try to stay in the business. Another conference, held in York in 1971, was also an eye opener for me. To be taught symbolic addition by Isabella Karle was memorable, as was meeting Edith Hauptman. Her opening words "Who is your father?" confused me until she explained how nice it must be to come to a meeting with one's parents. My students still benefit from my attendance at these early meetings; the chance to meet the people you've read about remains an exciting experience and the costs involved is money well spent.

In the spring of 1973, I left London for Munich on a Royal Society post-doc. My German had not improved but I managed to get to the little village of Martinsried without too much trouble. It was the weekend and the Max Planck Institute for Biochemistry was closed. I met two guards at the entrance, one of whom turned out to be a part-time bank robber. The latter was unusual and might have been more careful in his choice of cars since an E-type was an odd choice to find in these settings. Eventually he escaped from sunny Bayern but got homesick, returned, and was caught. The other guard was a friendly Corsican who I got to know quite well. The third person I met was Robert Huber. He showed me around, first taking me to the computer center. As we passed through the automatic door, a broad smile

Alwyn in the alps (a few years ago).

appeared on my face. A Siemens 4004 filled a very large room; the tyranny of the University Computer Center was over. It was a wonderful 9 months.

I was alone much of the time and RH took pity on me. I spent many a weekend scampering around the mountains with him and his young daughter, Ulrika, frantically trying to keep up with him. Of course, such trips always entailed a quick visit to the 4004 or the diffractometer. To slow him down, Ulrika and I would throw things at him but he was usually too fast for us, and out of range. Returning to London was an anti-climax, to say the least and my life proceeded to fall apart. There were two scientific bright spots. One was another trip to York, memorable for Michael Woolfson's imitation of an old testament prophet seeing the future of direct methods phasing macromolecular structures. The other was my first talk at a meeting, organized by Ulli Arndt and Allan Wonacott, in Groningen. With the likes of David Blow in the audience, my training at the COOP and in French lessons finally came into play. I met another "interesting guy" (how does crystallography manage this???) who looked like a front row forward, but with a strange accent. Paul Sigler and I drank a few beers together and he persuaded me that Chicago was the center of the world. I believed him; I like people with accents after all. I never made it though. Like in the Springsteen song, "I took a wrong turn and

I just kept going." Most London to Chicago flights do not go via Munich but mine did. Robert had no job to offer but suggested I talk to Johann Gassmann. Gassmann had been a former student of Walter Hoppe and was at the time in charge of the computer center, including the 4004 and some new items that he had just purchased and didn't know what to do with. I liked John; behind a rather severe exterior he was a great character. To everyone (except maybe Robert), he was Herr Gassmann, but to Peter Colman and me he was John. He was a bit competitive too which is always nice. He, or maybe Peter and I, challenged him to a game of doubles once. Of course, Peter and I hit every ball to his partner, and seeing John trying to cover the whole court remains an endearing memory. We won, by the way; more pizza to the workers. Peter was (is?) a pretty good player, but we have different memories of our singles games. Anyway, here I was back in John's office hearing about a Vector General 3400 computer graphics system that he had foolishly bought, and some money he had to pay someone to try to make it do something useful. So started the worst time of my life.

The 3400 was an amazing machine and a prototype. It was controlled by a PDP-11 and together cost as much as three Ferraris. It was, however, big and at least in those days you got some weight for your money. Programming such a system is a lot like trying to get my daughter's things packed into her room; no space. The computer program had to fit in 32k of 16-bit words, including the display list for the graphics system. The latter was in itself a computer program written in the machine code of the 3400. There was no space for a graphical API; I wrote the machine code instructions directly into the display list. This made debugging quite interesting, since an error in the machine code ended up with vectors getting interpreted as instructions and vice versa; the result was almost always an explosion of lines. The first year was very difficult but eventually I had a program that could do a few things. The PDP-11 was linked to the Siemens by a fast connection, so I had written a few programs to move the crystallographic data around. I had first read Lord of the Rings during my earlier trip to Munich, and it felt natural to name these programs after various characters in the book (data backwards and forwards --> circle -->ring). The graphics program was called Frodo or Sauron, depending on my mood.

Not knowing a subject is sometimes a good place to start from and I had another advantage, another Johann. Hans Deisenhofer had just solved the structure of Fc and wanted to refine it. He was willing to put up with a lot if it helped. He was a great guinea pig, although we had our moments, and I can still swear in his local dialect. John's money ran out after two years but Robert was able to keep me on for a third year. I had no future in Martinsried but good luck came in the form of Eila Zeppezaur (née Cedergren). Eila wanted to improve the model of alcohol dehydrogenase that had been solved in Uppsala, Sweden by Carl-Ivar Brandén and his co-workers. She came to Matrinsried and I helped her carry out the refinement. This in turn led to meeting Carl, Hans Eklund and an invitation to visit Sweden. It was early summer and lovely (they were careful not to invite me in November). Carl arranged a position for me, jointly with the other crystallography group in Uppsala, led by Bror Strandberg. I was the first thing they shared, and the second was a new graphics system. I was free to work on anything I wanted, and had a good time working on Bror's virus project with Lars Liljas and Torsten Unge. It was interacting with Hasse (Hans), though, that kept me through what was a big change. The curse of the University Computer Center returned, however, until Calle (Carl-Ivar) managed to get us enough money for our first Vax. What a difference 32 bits make to writing a program! Carl was great at getting money; I had wanted a color graphics system to allow me to develop some of my ideas and eventually we got an Evans & Sutherland PS330. I used these capabilities to implement a skeletonization / database approach to interpreting electron density maps and building models that I still use today.

My freedom allowed me to visit other labs, especially in November. You need to have lived through a few Nordic winters to understand the last sentence. At the beginning of November, you have to live through four months of even more darkness before it gets brighter than the November darkness; not nice. So my first November I spent in London as a house guest of Tom Blundell, getting Frodo working on the E&S PS2. Luckily Tom works long hours, and I was able to make a conversion in two weeks. But getting to know Ian Tickle and other members of his group was special for me. I well remember a young Lawrence Pearl getting me over to the student bar for a beer so that someone else could use the display.

My second November was even better. Michael Rossmann has a special attachment to Uppsala, and during a visit in 1980 he had made me an offer I couldn't refuse. As well as visiting Purdue in December, I'd visit St. Louis in November and Oregon in between. I didn't know America very well, so I thought it would be nicer than Uppsala, although I'd have to get Frodo running on another set of hardware, MMS-X. Before starting the trip, I got side-tracked into a visit to Boston too. In those days TWA had a great ticketing scheme, so provided I left from London, it would be rather cheap. Like the song, my journey started by train, then boat, then plane and I ended up in a depressed Boston on the first Tuesday after the second Monday of November or something, to a new President.

I had been invited to visit Harvard by Ian Wilson and to MIT by Greg Petsko. Ian was doing a post-doc with Don Wiley. I had seen Don at Alpbach and this was to be the first of many short interactions. My favorite was in Heidelberg, where we rescued Michael Levitt from potential disaster, but that's another story. My last sight of him was through the back window of a taxi, holding his wife, Kata's hand. His passing was a great loss to our community. Anyway, on to MIT. Greg had got a new graphics system and had heard that I could easily be persuaded to visit, but I arrived on a bad day. He had another visitor that he had to look after so he persuaded one of his hungrier graduate students to take me out for dinner. In those days, $20 was enough of a bribe if you'd not met the person in question. Greg is probably annoyed to this day that we didn't bring back any change. For the next seven years I tried hard to avoid meeting her; we got married in '88.

It was much harder to get Frodo working on the MMS-X system. It had been developed at Washington University in St.

Alwyn Jones and Sherry Mowbray with their children Elanor and Daniel Mowbray

Louis and been bought by a number of American macromolecular crystallographic laboratories. For me, it was a new graphics system and a new computer (a Texas Instruments 980). Fortunately a good linker was available from Colin Broughton who was working with Mike James' group. Colin was a remarkable character, and a great programmer. His molecular graphics program, M3, was used in Edmonton until their MMS-X disintegrated, and they still miss it. By the time I had to return to Sweden, Frodo was almost working and the finishing touches were made by Janet Smith (then working at the NRL with Wayne Hendrickson), for which I have been eternally grateful. The MMS-X conversion was a lot of work but the program did get used in a few laboratories during the 1980s, and I got the chance to make a lot of new friends. But it was exhausting and the last of my winter escapes.

I had learned a bit about how to write programs that were to be run on different computers and graphics systems. In 1986, I started putting this into practice, beginning afresh on a new program that was to become O. By this time, I had a couple of people working with me on solving structures, and I had no plan for making O available to others. I didn't have enough time to run a group, develop software and support a lot of users. It was meant as a little research project to make a program built on a simple database, with a minimalist set of tools that would help prevent making errors when building a model. The program was also designed to make it easy to add functionality without interfering with existing options. The latter became important when Morten Kjeldgaard from the University of Aarhus started working with me. This collaboration sometimes took the form of really enjoyable, short but intense trips, mostly to Uppsala. Our interactions lasted over a very happy ten years.

During this time, a rather tall Dutchman, Gerard Kleywegt, with a background in NMR came to do a short post-doc with me. This turned into a much longer stay and a collaboration that covered a broad range of subjects. Gerard arrived in Uppsala shortly after the birth of my first child, Daniel. I was spending less time in the lab, but found myself working with someone with remarkable ability. A suggestion made before rushing off to pick up Danny would result in something already done the next morning, and extended in ways that I had not foreseen. I can't say I'll never forget, but the memory of his many analyses of NCS related molecules, waiting for me each morning are still fresh. My favorite moments, though, were his introduction to Fourier calculations, and how appalled he was at the speed (or rather lack of it) of his first working algorithm. Also seeing how well ESSENS worked was particularly pleasing since it was one of the few "I told you so" moments I've ever had with him.

With Danny in a back-pack, Sherry and I could still go to meetings. He came to his first ACA meeting at 10 months, first CCP4 meeting at 16 months and Diffraction GRC at 22. Attending the Gordon Conference was a particular pain, since children were clearly not welcome. Two years later, though, we were back again. Michael Rossman saw us eating outside the dining room, in a cloud of mosquitoes. "Why are you sitting there, Alwyn?" he asked, "To feed the mosquitoes", I replied sarcastically. He was appalled that we were not allowed to eat in the canteen and stormed off to the GRC office. The young, but very tall man, in charge never had a chance. Calls were made, petitions drawn up and signed, visits made by GRC top-brass (just to ensure that we were not lowering the tone by too much), and we didn't have to sit outside anymore. Later the rules were changed, but we never went back. Elanor was born that autumn and I cut back as much as I could on traveling. There were a few notable exceptions, the XVII IUCr in Seattle being one of them. For us, even long meetings were not too exhausting since we only went to half of the sessions, but it seemed that in every conversation, the discussion was about the other session (I'm sure Sherry felt the same).

During the 90's, computers and graphics saw amazing advances. In the limited time available to me, I had the option of pursuing my development plans or supporting new hardware. I decided on the latter since I wanted a cheap computer on every student's desk. I moved over to Windows NT as soon as there was a good graphics card available, although it hurt to leave my lovely little Mac Duo. Gradually alternatives appeared in the shape of good quality cards that worked with Linux and Apple's OSX. Indeed, as soon as the first beta-release of OSX became available I bought a new Mac. The first program I started after the installation was, of course, Terminal, and then vi. Only this Christmas did I finish my low resolution building system, more than ten years after I had planned it. I am still working on my high resolution system although it's not clear if anyone other than me will find it interesting.

I was greatly honoured by the phone call from Frances Jurnak informing me that I was to receive the ACA Patterson award. The meeting itself was splendid, and reminded me how much I've missed attending the ACA. But you can't have everything. I brought the kids with me and while I enjoyed the meeting, they enjoyed the Disney attractions. They really want to go to Hawaii; it was clearly a mistake letting Elanor talk to Bill Duax at the banquet! Thanks to everyone I met in Orlando, it was wonderful.

Alwyn Jones

The Structural Genomics Consortium: new kid on the block

Structural genomics: Perspective: Structural genomics was born to anticipate the large numbers of proteins expected to be uncovered by genome sequencing efforts. Early structural genomics efforts set out to explore the use of different strategies and technologies in order to generate protein structural information at greatly reduced cost compared with any individual laboratory. In 2005, after many years of process development, the cost-per-structure has been driven down five-fold in many of the projects (in some cases down to $80,000 per structure); technology has been developed and transferred to the community; and some of the proteins whose structures were determined have been subsequently linked to human diseases.

Protein fold space: One objective of the larger structural genomics initiatives is to increase the understanding of protein structural space, and this goal is being accomplished. The ten-year Japanese initiative, which was launched in the late 1990's, has contributed 600 or so unique protein structures into the PDB. The Protein Structure Initiative of the NIH (PSI), which since 2000 has already placed more than 700 unique structures into the PDB, has now entered its second five-year phase, in which it plans to produce more than 1000 protein structures from unexplored Pfam families. The structures determined by world-wide efforts have provided the basis to infer the structures of over 40,000 relatives in the sequence databases. 45% or more of the unique structures in the PDB from 2000-2005 were derived from structural genomics initiatives ("unique"is defined as <30% identity to a protein with a structure in PDB).

Mammalian Proteins: Importantly, all of the structural genomics initiatives have placed significant emphasis on the development of new, enabling technology. These new capabilities spurred some of the projects to begin to focus on mammalian proteins. The largest number of structures determined derive from the Japanese initiative at RIKEN, which has, in addition to the structures from prokaryotic proteins, already deposited hundreds of mouse and human structures into the PDB. The scientific emphasis is on protein domains involved in signal transduction and protein-protein interactions. A large number of the structures were determined using NMR and from proteins produced in a cell-free system, attesting to the utility of this method, which was developed largely as part of their project.

In Europe, a consortium of investigators used funding from the European Union to develop formal ties among themselves under the umbrella of SPINE (Structural Proteomics IN Europe). SPINE investigators have worked to develop methods, to transfer technologies among members and to deposit the structures of mammalian proteins into the PDB. The SPINE investigators have placed emphasis on mammalian proteins, capitalizing on the expertise within the consortium.

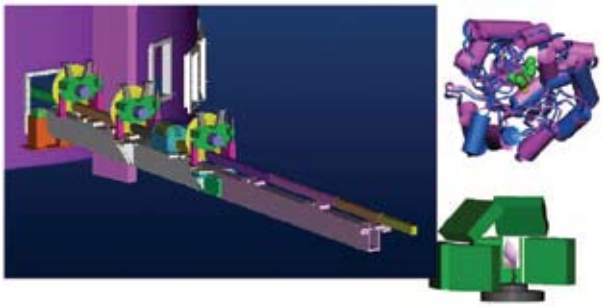
The newest structural genomics effort with a focus on mammalian proteins is the Structural Genomics Consortium (SGC). The SGC was created to substantially increase the numbers of structures of human therapeutic targets in the public domain, free from restriction on use. The SGC operates from laboratories at the Karolinska Institutet (Stockholm) and the Universities of Oxford and Toronto and works from a confidential list of 2,000 targets created / approved by a Scientific Committee, which is composed of independent scientists selected by the funders of the consortium. The SGC target list is confidential, but not the general areas of scientific interest, which can be found on the SGC web site (**www.thesgc.com**).

The SGC was funded to work toward quantitative obvjectives, and was mandated to determine the structures of 50, 100 and 200 proteins from the Target List in its first three year of operations, respectively, beginning in July, 2004. In 2005, the SGC contributed 152 structures into the PDB (at a cost of ~$125,000 per structure). Highlights of the SGC science in 2005 include: completing the structural descriptions of three human protein families: cytosolic sulfotransferases (10 structures, 5 done by SGC), the human adenylate kinases (6 structures, 5 done by SGC) and the human 14-3-3 proteins (7 structures, 5 done by SGC); three different structures of two ion channels; and many structures of proteins that are existing drug targets or for which there are compounds in clinical development.

In summary, structural genomics projects around the world continue to develop technologies and methods to reduce the cost of structure determination and increase the breadth of the proteins that are amenable to the methods. The efforts are now being focused on human proteins, with early signs of success.

Aled Edwards

The Future of Neutron Crystallography: A New Macromolecular Neutron Diffractometer (MaNDi) at the Spallation Neutron Source (SNS)



Neutron Macromolecular Crystallography (NMC) can fill an important niche in structural biology, enzymology, and functional genomics due to its versatility in the accurate determination of protons, protonation states, and hydration in macromolecular crystals even at a moderate 2.0 to 2.5 Å resolution.[1] Although ultra-high resolution x-ray crystallography (UHRXMC) at third generation synchrotron sources can locate some of the more ordered hydrogen atoms on cryo-protected, highly-ordered protein crystals,[2] and determine the protonation states of amino acid side chains,[3] there are many instances where the information obtained remains inadequate. For instance, in myoglobin, even at resolutions better than 1.15 Å, UHRXMC did not provide hydrogen positions,[4] whilst NMC on perdeuterated protein enabled the same hydrogen atom positions to be visualized in a structure determined to 2.0 Å resolution.[5]

The knowledge about protonation states of amino acid residues in the active sites of enzymes is crucial for an understanding of reaction mechanisms. Identification of protonated amino acids in the catalytic center can make it possible to discriminate between two or more competing reaction models.[6] In trypsin, this type of critical information from NMC helped to resolve the question about which of the two amino acids, Asp-102 or His-57, is the origin of the catalytic proton.[7]

Even though NMC is a powerful technique, its productivity has been severely constrained by the scarcity of facilities and the intrinsic low brightness of available neutron sources. Currently there are only a very limited number of instruments that are recognized to be useful for high resolution single crystal macromolecular neutron crystallography: LADI at the Institut Laue-Langevin (ILL), Grenoble, France; BIX3/BIX4 at the Japan Atomic Energy Research Institute (JAERI), Tokai; and PCS at Los Alamos National Laboratory (LANL). While the reactor based LADI and BIX3 instruments were operational during the past five to seven years, the time-of-flight diffractometer PCS at the spallation source at LANL has only become available during early 2002.

With the advent of the SNS at Oak Ridge National Laboratory, an excellent opportunity exists for the development of a powerful high resolution neutron diffractometer for structural biology. SNS will produce more than an order of magnitude higher intensity than the Los Alamos facility, and the opportunity exists at SNS to design a fully optimized diffractometer for NMC. Furthermore, cryogenic moderators, state-of-the-art neutron guides, and high sensitivity, high resolution detectors should allow additional factors of increased data rates and improved resolution to be realized.

Toward these ends, we have developed a conceptual design for a dedicated, best-in-class and high resolution, time-of-flight, single-crystal, macromolecular neutron diffractometer (MaNDi) at the SNS high-power target station (HPTS) which operates at 60 Hz. Design calculations, using analytical expressions and Monte Carlo simulations, show that the data rates at the MaNDi instrument can be over 50 times greater than at currently available sources.[8] Thus, it will be possible to investigate larger unit cell systems at high resolution, using smaller crystals. It is expected that the unprecedented high data rates and resolution with MaNDi will revolutionize NMC and greatly advance the field of structural biology.

We encourage you to attend the 2006 ACA meeting in Hawaii which will feature a *Transactions* Symposium on "The Future of Neutron Crystallography: Smaller Crystals, Larger (Macro) Molecules" and to participate in the workshop on "Methods in Neutron Protein Crystallography". (see p. 35.) For more information on MaNDi, please consult **pns.anl.gov/instruments/mandi/mandi.html**; and **sns.gov/workshops/mandi2005/**.

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1. Wlodawer, 1982; Wlodawer & Hendrickson, 1982; Kossiakoff, 1983; Kossiakoff, 1984; Schoenborn, 1984; Wlodawer et al., 1984; Borah et al., 1985; Kossiakoff, 1985; Schoenborn, 1985; Raghavan & Wlodawer, 1987; Wlodawer et al., 1989; Timmins, 1995; Schoenborn, 1996; Helliwell, 1997; Niimura et al., 1997; Bon et al., 1999; Niimura, 1999b; Habash et al., 2000; Shu et al., 2000; Coates et al., 2001; Gutberlet et al., 2001; Ho et al., 2001; Kurihara, 2001; Ostermann et al., 2002; Tsyba & Bau, 2002.

2. Longhi et al., 1997; Kuhn et al., 1998; Jelsch et al., 2000.

3. Berisio et al., 1999.

4. Kachalova et al., 1999; Vojtechovsky et al., 1999; Miele et al., 2003.

5. Shu et al., 2000.

6. Schmidt et al., 1996.

7. Kossiakoff & Spencer, 1981.

8. A. J. Schultz, P. Thiyagarajan, J. P. Hodges, C. Rehm, D. A. A. Myles, P. Langan and A. D. Mesecar. "Conceptual design of a macromolecular neutron diffractometer (MaNDi) for the SNS". J. Appl. Cryst. (2005), 38, 964-974.

"Physics at the farm: discovery of the muon" by Nick D. Kim, U. Waikato, New Zealand. See nearingzero.net/res.html.

The Theory of Almost Everything: The Standard Model, the Unsung Triumph of Modern Physics,

by **Robert Oerter**, Penguin Group USA, (2005), hardcover, 336 pp. $16.47, ISBN: 0-132-36678-9.

Robert Oerter teaches particle physics at George Mason University; has done research in supergravity theories including quantum chaos and string theory and has a particular interest in the foundations of quantum mechanics. Oerter writes with clarity about the "Standard Model" which was put together in the 70s to combine the relativistic quantum field theories of quantum electrodynamics (QED) and quantum chromodynamics (QCD) and which explains all the interactions of all the elementary particles ever observed plus the one remaining particle predicted (the Higgs) that has not yet been observed. The Standard Model is considered to be a huge success because it has predicted, with spectacular precision, so many particles that were then subsequently found. (Within the next few years, either Fermilab's Tevatron accelerator or the Large Hadron Collider (LHC) now under construction at CERN may well find the Higgs.)

What the Standard Model does NOT do is explain the relationship of gravity to the other forces, or account for 85% of the matter in the universe (dark matter), or offer clues about why the universe seems to be expanding at an accelerating rate (dark energy?). In his final chapters, Oerter lays out in a practical way the questions that need to be answered and the directions that theoretical physics may take, *i.e.* theories with more *symmetry* such as Grand Unified Theories (GUTs) with and without supersymmetry, and theories with *deeper structure* (preons, string theory).

The three appendices give details about the structure of quarks; the relationship between the color force and energy and distance; and the Feynman diagrams for the Standard Model, showing all interactions among all elementary particles. One deficiency is that there is no index, making it difficult to find answers to specific questions. The book is nevertheless a welcome addition to the current collection of physics-for-the-layman books because it is very easy to read and because the analogies Oerter uses are appropriate and helpful.

Warped Passages: Unraveling the Mysteries of the Universe's Hidden Dimensions, by **Lisa Randall,**

HarperCollins Publishers, New York, NY (2005), hardcover, 499 pp. $27.95, ISBN: 0-06-053108-8.

Lisa Randall is a professor of physics at Harvard, and is the winner of an Alfred P. Sloan Foundation Fellowship and a NSF Young Investigator Award.

Warped Passages is a treat to read; Randall explains lucidly and with clever analogies where we are currently with the theoretical physics that attempts to explain our universe and then goes on to describe her own intriguing research into extra warped dimensions. Two papers published with Raman Sundrum of Johns Hopkins University brought her acclaim and respect from the physics community because they describe how warped space could explain why gravity is such a feeble force. (The "hierarchy" problem – why the force of gravity is so weak compared to the non-gravitational forces - is regarded as one of the most puzzling problems in physics.) The papers present two new Kaluza-Klein scenarios, concentrating on a five-dimensional spacetime in which gravity is localized in a small region. Randall describes a "brane" as a "distinct region of spacetime that extends through only a (possibly multidimensional) slice of space." The first Randall & Sundrum paper postulates a two brane model; the second a single reflective brane sitting at one end of the fifth spacetime dimension; the Standard Model particles are confined there, and whatever hits the brane simply bounces back so that no energy is lost. In this scenario the graviton would have unrestricted access to the fifth dimension, but would be highly concentrated in the vicinity of the brane. If indeed the universe has 10 or more dimensions, then some mixture of localization and curling up hides the additional dimensions, but these would not affect this localization phenomenon. One very exciting thing about Randall's ideas is that some of them may actually be tested very soon (by experiments at the Large Hadron Collider at CERN). (Supersymmetry will also be tested at the LHC and she thinks that supersymmetry is not necessarily incompatible with warped extra dimensions.) Lisa Randall describes herself as an agnostic where string theory is concerned, but says her research into string theory has provided much of the impetus for her study of extra dimensions. Her book is all the more readable for the personal touches included.

Out of Gas: The End of the Age of Oil, by **David Goodstein,** Norton, W. W. & Company, Inc.,(2005) paperback, 149 pp. $13.95, ISBN: 0-39-332647-0.

David Goodstein is vice provost and Frank J. Galloon Distinguished Teaching and Service Professor at Caltech. He also wrote *Feynman's Lost Lecture*, among other works.

Out of Gas is a quick read at 123 pages (plus a Postscript to the paperback version; Notes; Annotated Bibliography; and an index). It is an incisive and sobering warning that "Civilization as we know it will come to an end sometime in this century unless we find a way to live without fossil fuels." His arguments are based solidly on the laws of physics, and go like this: "In the 1950s, Shell Oil Company geophysicist M. King Hubbert predicted that the rate at which oil would be extracted from wells in the United States would peak around 1970 and decline rapidly after that." This forecast was disparaged at the time, but turned out to be correct and Hubbert's methods have been used by oil companies ever since as a way to predict future yields. Data analogous to that used to predict "Hubbert's peak" for the US is now available for the entire world, and while estimates differ because of disagreements about the total amount of oil and other numbers, there is not much doubt that the world-wide Hubbert's peak could occur within the next decade, and, even using quite optimistic numbers, will occur within the next two or three decades. The take-home lesson is that "*the crisis will come when we have used about half the oil nature made for us*."

Despite all this, Goodstein is no doom and gloom preacher; he manages to give the reader a silver lining in that if we are able, by scientific ingenuity and dedicated hard work, to kick our fossil fuel habit, then we may well prevent a fate far worse than serious enonomic trouble: "irreversible damage to the climate of the only planet we have."

Highlights from the 63rd Annual Pittsburgh Diffraction Conference

Argonne National Laboratory, 3-5 November, 2006

Pittsburgh Diffraction Society Past- President Alan Pinkerton presenting the Sidhu Award to Chong-Yu Ruan.

This year the **Sidhu Award** "for a scientist within five years of the Ph.D. who has made an outstanding contribution to crystallography or diffraction" was made to **Chong-Yu Ruan**, Assistant Professor of Condensed Matter Physics at Michigan State University. The award was made based on his work in ultrafast electron diffraction and ultrafast electron spectroscopy. In his presentation he discussed this methodology with respect to the transient structure of molecules on surfaces, and new capabilities with respect to spatial and temporal resolution.

The **Chung Soo Yoo Award** "to a graduate student presenting the best poster at the annual conference" was shared by **Stacy Gates** from the University of Toledo for her poster *High Pressure In Situ Diffraction Study of Gallium Molybdenum Oxide,* and **Eric J. Yearley** also from the University of Toledo, for his poster *Preliminary Results of the Recent Charge Density Study of Genistein.*

The opening symposium, ***X-rays, Crystals, and a Life: Through the Looking Glass of Leroy Alexander,*** organized by **Jim Kaduk** and **Bob Von Dreele**, began with a survey of his work by one of his collaborators, **Gordon Smith**, and continued with a series of talks that gave some modern extensions. **Cam Hubbard** reviewed the neutron instrumental requirements for residual stress measurements and pointed out the very high precision and accuracy needed for this work. In a similar vein, **Pam Whitfield** presented the issues in accuracy for quantitative phase analysis by the Rietveld method on x-ray powder diffraction data with particular emphasis on systematic effects from microabsorption. As a bow to Alexander's later work, **Peter Stephens** showed the current slippery status of the silver behenate structure and **Christian Burger** showed how diffraction studies of polymer fibers can give information about their texture/preferred orientation. The session closed with an oral presentation by **Stacy Gates** of her poster on pressure induced phase changes for the negative thermal expansion material, $Ga_2Mo_3O_{12}$.

Friday's program featured a symposium on ***Frontiers in Neutron Scattering***. This was followed by tours offering conference attendees an opportunity to visit the research facilities at the Intense Pulsed Neutron Source or at the Advanced Photon Source. **A. Albinati** kicked off the morning session by summarizing the contributions of neutron diffraction in a broad range of studies to probe the coordination chemistry of hydrogen. **J. Eckert** then described recent contributions that he and his collaborators have made to understanding the complex behavior of very short, intramolecular hydrogen bonds by combining neutron diffraction with inelastic scattering and *ab initio* calculations. **M. Christensen** presented results of his studies of some semiconducting clathrates that possess interesting thermal conductivities or magnetic properties, and **J. Parise** closed the morning session with an overview of the extremely exciting area of neutron diffraction studies of materials at high pressure.

To open the afternoon session, neutron protein crystallography was featured in a presentation by **A. Podjarny** who discussed new results on the structure and mechanism of action of AR - human aldose reductase. The enzyme AR has been studied by ultra-high resolution synchrotron x-ray diffraction as well as by neutron diffraction using fully deuterated crystals. By combining results from the two techniques, unique insights have been obtained regarding the protonation states of key residues in the region of the active site. Following Podjarny's presentation, **P. Thiyagarajan** described the use of small-angle scattering to study the pH-dependent self-assembly of a β peptide, the primary constituent of amyloid plaques found in the brains of Alzheimer's patients, into fibrils and charged

The Chung Soo Yoo award presentation by Alan Pinkerton to Eric Yearley and Stacy Gates.

nanotubes. **D. Worcester** outlined the use of grazing-incidence neutron diffraction, in conjunction with deuterium labeling, to study nanoscale structural features in highly oriented multilayer membranes of phospholipids and cholesterol. The symposium closed with a student presentation by **E. Yearley** discussing the charge-density of the nonsteroidal phytoestrogen, genistein, which formed the subject of his poster at the conference.

The 1999 Pittsburgh Diffraction Conference at Ohio State University was organized to honor Dr. Muttaiya Sundaralingam upon his retirement. This year's special ***Sunda Symposium*** at the Pittsburgh Diffraction Conference at Argonne was organized in Sunda's memory following his tragic death, together with his wife Indrani, in the great tsunami of December 26, 2004 (see N. Yathindra, *Acta Cryst.* **D60**, 845-849, 2005). At the time Sunda was on vacation in his homeland of Sri Lanka. The symposium

included presentations from Sunda's students who shared their graduate careers in his laboratory at the University of Wisconsin in Madison during the 1970s. The purpose of the morning session was to demonstrate that at one time Sunda's lab harbored a unique collection of students, who have continued to do a wide variety of crystallographic research, all connected in some way to the inspiration he provided. This on-going research, which Sunda initially mentored, was presented as a testimony to his contribution to crystallography. Six former students attended the symposium. **Jim Hogle** presented his work toward understanding the molecular life cycle of polio virus in his talk, *On the Outside Looking in: A Multiscale Approach to Characterizing Poliovirus Cell Entry*. **Ethan Merritt** spoke on *Protein Structures As Blurred Snapshots – Extracting Dynamic Information From A Static Experiment*, and described a greatly improved method for extracting TLS parameters for protein refinement. **Janet Smith** described the design and commissioning of three new NIH sponsored beamlines at Sector 23 of the Advanced Light Source. Her talk was titled *GM/CA Canted Undulator Beamlines for Macromolecular Crystallography*. **Steve Sprang** talked on *Regulating G-proteins with Peptides: Mechanistic Insights from Unexpected Sources*, and described several crystal structures of signal transducing molecules in complex with effector proteins and peptides mimicking the larger proteins. **Dave Stout** talked on the *Structure and Function of Transhydrogenase*, summarizing experiments to understand the mechanism of this integral membrane protein, proton pump, and respiratory complex of mitochondria. **John McAlister** also attended the symposium. Sunda's family, through his son Rohan, is working to establish a foundation that will support a memorial award, lecture, or meeting in their father's memory.

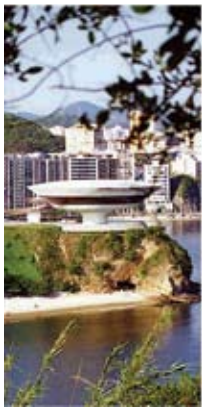
The final session of PDC '06 was on ***Advances in Chemical Biology.*** The session featured a cross section of various structural approaches, structure based drug-design and the Laue method for kinetic studies, as well as systems of interest, the haloalkanoate dehalogenase superfamily and protein complexes involved in the bacterial chemotaxis process. **Charles Eigenbrot** led off the session with an example of the application of structure based drug design to the synthesis of an active site inhibitor of the serine protease factor VIIa. The factor VIIa in complex with its cofactor tissue factor initiates blood coagulation. **Karen Allen** followed with her work on the haloalkanoate dehalogenase superfamily (HADSF). This superfamily consists of a majority of members that are phosphotransferases. The structure of a ß-phosphoglucomutase with a Mg cofactor and substrate revealed a stabilized pentavalent phosphorane. This trapped intermediate has led to kinetic studies to elucidate the details of the mechanism of phosphoryl transfer and suggestions about the dissociation and rebinding of the substrate. Karen extended the reaction mechanism to the role of the HADSF superfamily protein domains. The third speaker of the session was **Brian Crane**, who discussed how the biology of bacterial chemotaxis -basic chemical biology- was examined through structures of the receptor cytoplasmic domain, and the histidine kinase (CheA) – adaptor protein (CheW) complex. These three components regulate motility of the bacteria in response to the change in the chemical environment. The structures were used to build a plausible model for the explanation of CheA/W-dependent clustering of receptors and their functioning in signaling. Finally, **Keith Moffat** introduced the technique of Laue diffraction applied to photochemical systems. Using the method of singular value decomposition on time resolved data he followed the changes in the Photoactive Yellow Protein (PYP). The results showed not only the isomerization of the chromophore at the active site but also the slower propagation of changes throughout the chromophore. This was the last presentation of the day, and an extensive and lively discussion of the results brought the session and the meeting to a close.

The poster session on Thursday evening included presentations on new techniques in macromolecular crystallography by **M. Benning** and **C. Bauer** of Bruker AXS, who described the collection of high-resolution data in a home x-ray lab, and by **A. Criswell** and co-workers from Rigaku/MSC on automatic crystal-screening procedures developed for use in high-throughput experiments. A poster on human aldose reductase by **A. Mitschler** *et al.* complemented A. Podjarny's talk in Friday's *Frontiers in Neutron Scatttering* symposium. **K. Shi** presented work carried out in the Ohlendorf Group on tetrameric PrgX, a key player in controlling conjugation induced by the peptide pheromone cCF10 in *Enterococcus faecalis*, which is elucidating the control mechanisms that operate in this system. Four additional posters were presented by IPNS staff members. These included powder diffraction studies by **A. Huq** *et al.* on two interesting materials: ferric molybdate and ferric molybdate/bismuth molybdate mixtures, which are model ammoxidation catalyst sytems, and $YbBaCo_4O_7^{+x}$, a transition metal oxide material that exhibits interesting physics with structural and magnetic phase transitions. **T. Koetzle** *et al.* presented recent single-crystal neutron diffraction results from IPNS on transition metal σ complexes. Developments on MaNDi - the macromolecular neutron diffractometer that is currently under development for the Spallation Neutron Source (SNS) - were presented by **A. Schultz** *et al.* Two interesting student posters by **S. Gates** and **E. Yearley** complemented their contributions to the oral program. Finally, in a late addition to the poster session, **C. Hoffmann** *et al.* described Topaz - the single-crystal neutron diffractometer under construction at SNS that is scheduled to be operational in 2009.

Tom Koetzle, Alan Pinkerton, Robert Von Dreele, Craig Ogata, & Charles Stout

Paula Piccoli (on the left) and Ashfia Huq
Photos are courtesy of Merlyn Faber of Argonne IPNS.

Crystallography Symposium at Universidade Federal Fluminense



Brazil has a number of x-ray laboratories and research centers dedicated to the study of the structure of matter. These include a National Synchrotron Radiation Facility, and the Laboratório Nacional de Luz Síncrotron (LNLS) located in Campinas, SP. Nevertheless, until recently, the State of Rio de Janeiro did not have an x-ray laboratory with the infrastructure required to study single crystals.



Glaucius Oliva (IFSC-USP); the audience; and Ademir Neves, UFSC. All photos courtesy of Iris Torriani.

A consortium recently formed by researchers from the Univ. Federal Fluminense (UFF) and other universities and research institutes in the State of Rio de Janeiro, has made possible the installation of a new x-ray diffraction facility. X-ray equipment has been acquired for several applications, such as small molecule structure solution and the study of polycrystalline materials. The aim is to satisfy the interests of all those involved in the newly formed LDRX Laboratory at the UFF and to attract new students to this area of research.

For the inauguration of the LDRX-UFF a symposium was organized at the Universidade Federal Fluminense, Campus Praia Vermelha, Niteroi, RJ. The symposium featured lectures covering such subjects as: small molecule structures and drug design; crystallography of organometallic compounds and clusters; protein crystallography; x-ray powder diffraction and the Rietveld method; x-ray diffraction as an analytical tool; the study of phase transitions; the structure of thin films and the applications of XRD in metallurgy.

The symposium was very successful, the participants (more than 150) were young students and researchers from the physics, chemistry, biology and engineering schools of the UFF as well as other universities and research institutions of the State of Rio de Janeiro. The Organizing Committee members were: Carlos B. Pinheiro (IQ-UFF), Maria G.F. Vaz (IQ-UFF), and Renato B. Guimarães (IF-UFF)

Iris L. Torriani, Rio de Janeiro

Intercontinental Collaboration in the Southern Hemisphere:

L to R: DT Britton (UK), Tshepo Ntseone (South Africa), Ziyanda Sigcau (South Africa), Fhatuwani Nemalili (South Africa), Fhatuwani Ramukosi (South Africa), M Harting (Germany), Evariste Minani (Rwanda), Iris Toriani (Brazil), Christiano Olivera (Brazil), Schadrach Nsevgiyumva (Rwanda), Odo Ayodele (Nigeria), Girma Goro Gonfa (Ethiopia).

During the last two weeks of November 2005, a team from Cape Town University, South Africa visited the Brazilian Synchrotron Radiation Facility for the use of three beamlines: XRD2 (high resolution XRD), XPD (powder diffraction) and SAXS1 (small angle x-ray scattering). For the leaders of the team, David T Britton and Margit Harting, from the Department of Physics (CTU), this was the second visit to LNLS since 2003. They have developed a program of basic and applied research on amorphous and nanocrystalline hydrogenated silicon within the scope of the South African Nanotechnology Initiative.

Iris L. Torriani

Contributors to this Issue:

Sidney Abrahams, Frank Allen, Bob Bau, Patrick Carroll, Marcia Colquhoun, Bryan Craven, Louis Delbaere, Howard Einspahr, Alwyn Jones, Lisa Keefe, Judy Kelly, Thomas Koetzle, Charles Lake, Charles Majkrzak, Andrew Mesecar, Dean Myles, Craig Ogata, Alan Pinkerton, Miriam Rossi, Amy Sarjeant, Arthur Schultz, Karl Seff, Charlie Simmons, Charles Stout, P. Thiyagarajan, Iris Torriani, Robert Von Dreele.

ACA 2006 July 22 – 27 Sheraton Waikiki, Honolulu, Hawaii

Advance Registration Deadline: June 1, 2006

Advance Hotel Registration Deadline: June 13, 2006

The Call for Papers, on-line abstract submission instructions, on-line registration, and a preliminary meeting program are posted on the ACA website at: **hwi.buffalo.edu/ACA/**. The 2006 ACA meeting will begin with workshops on Saturday, July 22. Symposia and sessions will begin on Sunday morning, July 23. Consult the Call for Papers for detailed information on workshops and sessions. Meeting website: **xray.chem.ufl.edu/aca2006/index.html** ***ALOHA!***

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Photos are courtesy of the Polynesian Cultural Center.

Symposia:

Transactions **Symposium: Neutron Diffraction (featuring its uses in studying biological macromolecules as well as small molecules and recent developments in neutron techniques), organized by Tom Koetzle, Paul Langan, and Alberto Podjarny.**

Buerger Award Symposium to honor Helen Berman, 2006 Awardee.

Warren Award Symposium to honor Charles Majkrzak, 2006 Awardee.

Etter Award Symposium to honor Carrie Wilmot, 2006 Awardee.

Workshops:

The Management of Synchrotron Image Data: The imgCIF File System and Beyond, organized by the Data, Standards and Computing Committee.

An Introduction to Grazing Incidence Small Angle Scattering with X-rays and Neutrons, organized by the Small Angle Scattering SIG, Chairs: R. Winans and Jin Wang.

Methods in Neutron Protein Crystallography, organized by Neutron Diffraction SIG, Chairs: Paul Adams and Paul Langan.

Sampling of Scientific Sessions:

Whole-Molecule Disorder, PDF Analysis of Industrially Relevant Materials, Detectors, Solving Difficult Organics and Organometallics, Macromolecular Assemblies, Non-Ambient Crystallography, Structural Genomics, Natural Products and Drugs, Polymer Science and Technology, Computational Methods, Proteins Involved In Immune System /Pathogen Interactions, Crystal Engineering, Time Dependent Investigations, Membrane Proteins, Pair Distribution Function Analysis and Small Angle Scattering, Radiation Damage.

New: Undergraduate Research Showcase

This symposium will feature oral presentations and posters presented by undergraduates on their crystallographic research, as well as oral presentations by mentors on research programs and programmatic developments at predominantly undergraduate institutions.

New Photo Contest: Entries to a Photo Contest – Sponsored by Crystal Growth & Design – will be displayed at the Meeting. The deadline for email entries is June 23, 2006. See the ACA website hwi.buffalo.edu/ACA/ for details.

APRIL 2006

23-28 **RapiData 2006 - Rapid Data Collection and Structure Solving at the NSLS: A Practical Course in Macromolecular X-Ray Diffraction Measurement.** NSLS, Brookhaven National Lab, NY.

24-28 **Practical X-Ray Fluorescence**, ICDD School, Newtown Square, PA.

25-26 **Advances in Functional Genomics,** South San Francisco, CA.

MAY 2006

8-10 **6th Canadian Powder Diffraction Workshop.** U. Waterloo, Ontario, Canada.

18-26 **LANSCE Joint School in Neutron Scattering in Soft Condensed Matter and Structural Biology;** Neutron Scattering Center, LANL, Los Alamos NM.

JUNE 2006

1-3 **36th Mid-Atlantic Macromolecular Crystallography Meeting.** Wake Forest Univ., Winston-Salem, NC.

5-9 **Fundamentals of X-Ray Powder Diffraction**; ICDD School; Newtown Square, PA.

9-18 **Structural Biology of Large Molecular Assemblies**; 38th crystallographic course at the Ettore Majorana Centre, Erice, Italy. **www.crystalerice.org/futuremeet.htm**

12-16 **Advanced Methods in X-Ray Powder Diffraction**; ICDD School; Newtown Square, PA.

18-22 **ACNS 2006 - 3rd American Conference on Neutron Scattering.** Pheasant Run Conference Center, St. Charles, IL.

JULY 2006

22-27 **ACA Annual Meeting, ACA 2006,** Sheraton Wakiki, Honolulu, Hawaii. **www.xray.chem.ufl.edu/aca2006/index.html**

AUGUST 2006

4-6 **ECM-23 Satellite Meeting on Mathematical and Theoretical Crystallography.** Leuven, Belgium.

6-11 **ECM 23 - 23rd European Crystallographic Meeting.** Leuven, Belgium.

OCTOBER 2006

22-26 **4th International Conference on Structural Genomics**. Beijing, China. **www.sino-meetings.com/icsg2006/**

JUNE 2007

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

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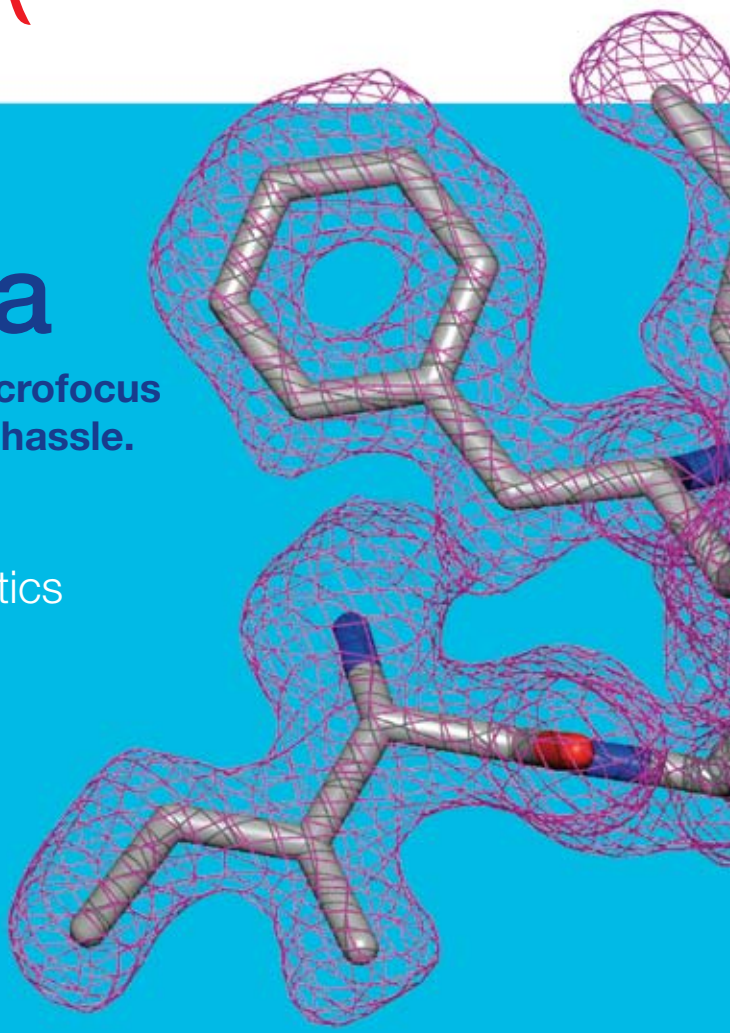

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