American Crystallographic Association

NEWSLETTER

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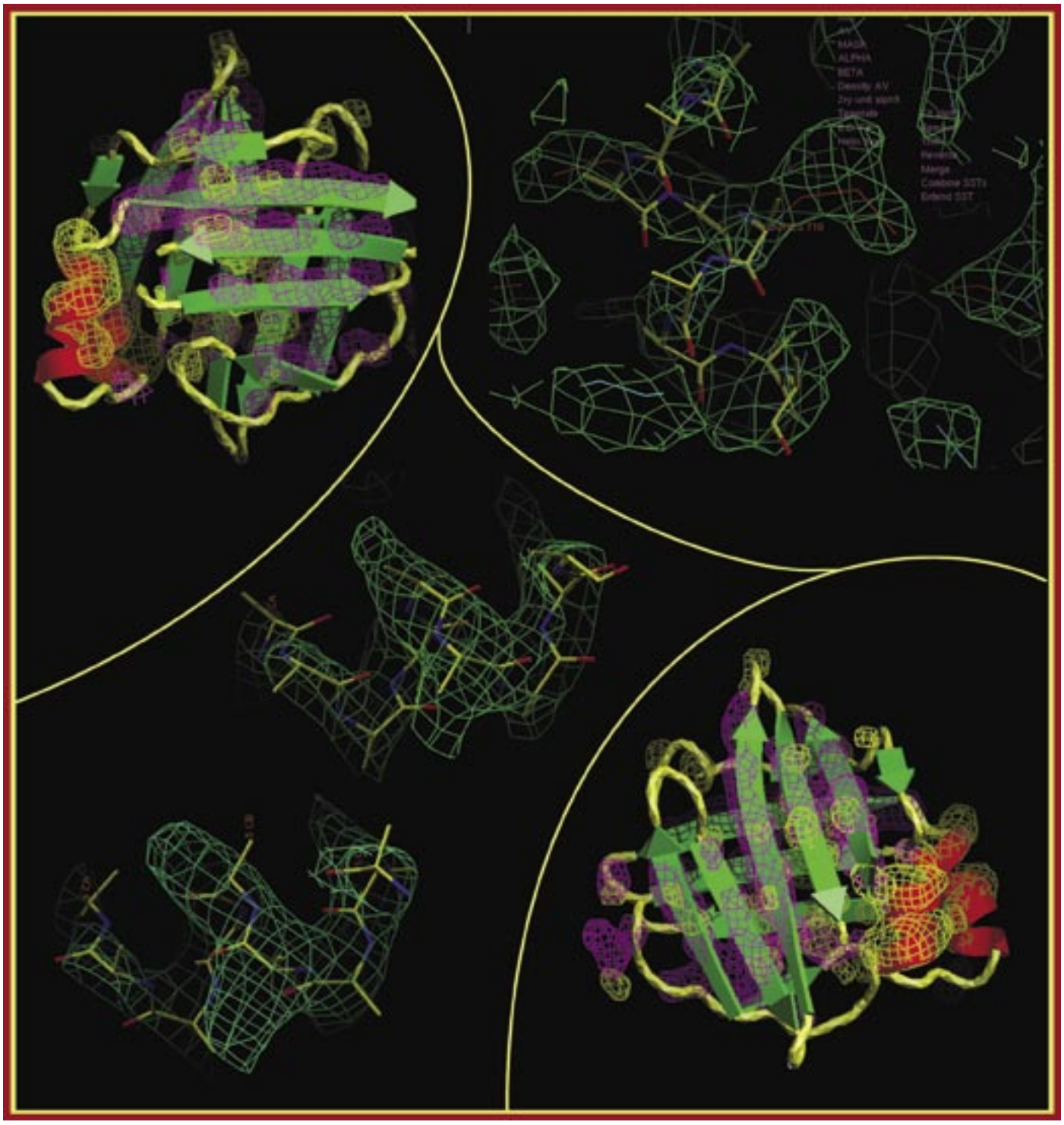

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President's Column

I must begin on a sad note because the crystallographic community has suffered a great loss with the death of Muttaiya Sundaralingam and his wife, Indrani. They were vacationing and visiting friends in Sri Lanka and were staying in a beach town where they were among the casulties when the tsunami struck. Their daughter and her family were on vacation with them, but were spared because they had traveled to Colombo. Our sincere sympathy goes out to the entire Sundralingam family and to all his many students.

In this my inaugural message I invite all ACA members to attend the Annual Meeting in Orlando, Florida from May 28th to June 2nd at the Walt Disney World Swan Hotel. There will be excellent science presented and you will be able to meet old friends as well as make new ones. The Annual Meeting is early this year because the IUCr meeting in Florence, Italy will be August 23 - 31, and many of our members are likely to attend both conferences. Our 2006 ACA Annual Meeting will also be in a beautiful location; we will meet at the Sheraton Waikiki Beach Hotel in Honolulu, Hawaii, July 22-29, 2006.

In order to encourage participation of Central and South America in the ACA, the Latin America Country membership has been developed (led mainly by Bill Duax, our CEO and the President of the IUCr). A certain amount of travel support to attend ACA meetings is available for leaders and students from these national crystallographic associations. Individual crystallographers from all Latin American countries are also encouraged to apply for ACA membership.

Volunteers are very important for the success of the ACA. I would like to thank all volunteers for their valuable work, including our Annual Meeting Local Chairs (Khalil Abboud and Tom Selby in 2005) and Program Chairs (Ed Collins in 2005), our *Newsletter* Editors (Connie Chidester and Judy Flippen-Anderson), members of Council, and members and officers of our SIGs and Standing Committees. I would especially like to thank Ray Davis and David Rose for their contributions, as they leave their positions of Past President and Canadian Representative, respectively, on Council; we have greatly appreciated their thoughtful assistance in discussions. I would also like to welcome Robert Bau and Lee Groat as new members on Council, Vice President and Canadian Representative, respectively. Our appreciation also extends to the excellent staff at the ACA office in Buffalo (Marcia Colquhoun, our Director of Administrative Services, and Patti Coley and Tammy Colley), as they continue to enable the annual meetings and our association to run efficiently and smoothly.

continued on page 4

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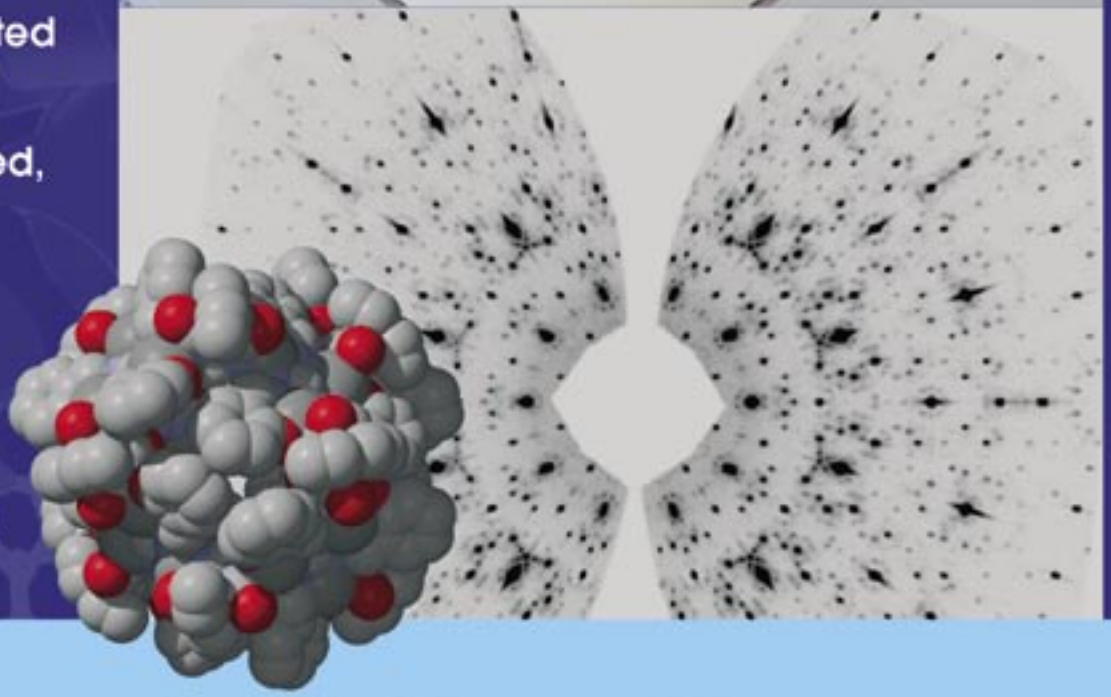

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President's Column, con't

The 2005 Etter awardee is Jennifer Swift who will receive the award in Orlando and will give a presentation in a session organized by the Young Scientist and General Interest Group SIGs. The 2005 Patterson Award will honor Alwyn Jones, who revolutionized the use of computer graphics in protein structure determination. Alwyn will receive the award and give a presentation in Orlando at the A.L. Patterson Symposium on Macromolecular Model Building and Validation organized by Gerald Kleywegt.

The ACA Awards scheduled for selection this year are the Buerger, Warren and Etter Awards. The Call for Buerger and Warren nominations was in the fall 2004 *Newsletter*. The Call for nominations for the Margaret C. Etter Early Career Award was in the winter 2004 issue and is also elsewhere in this *Newsletter.*

Louis Delbaere

Structural Biology; Past, Present, and Future, a Guest Editorial by Jill Trewhella

After 20 years at Los Alamos that she enthusiatically describes as "wonderful," Jill Trewhella recently moved her laboratory to the Chemistry Department at the University of Utah. This coming July, she will be taking up her appointment as Professor of Microbial and Molecular Bioscience and Australian Federation Fellow at Sydney University, with a joint appointment at ANSTO's Bragg Institute. She plans to split her time between Australia and the US, continuing her research on the structural biology of second messenger mediated signaling.

During these first few years of our new century, we have been witness to a number of anniversaries of epoch making breakthroughs in our understanding of the structures of the molecules of life. An obvious stand out was the widely celebrated 50th anniversary of the publication in *Nature* of the double helical DNA structure and related papers by Watson, Crick, Wilkins, Stokes, Wilson, Franklin, and Gosling in 1953 which led to the central dogma that drove much of 20th century molecular biology; information is stored in DNA sequences and translated via RNA into functional proteins. In 2004, one year after DNA was the dominating science "story," there were more modest celebrations to mark the 50th anniversary of the publication, again in *Nature,* of the sliding filament model of muscle contraction by two independent groups; Huxley (H.) and Hansen, and Huxley (A. F.) and Niedergerke. Huxley and Hansen went further in their paper and identified the thin and thick filaments of striated muscle with the then known molecular components, actin and myosin, respectively. This work has provided the framework for probing the molecular mechanisms underlying motility in biology.

It is interesting to reflect on the parallels and distinctions in how these stories unfolded. Each had at their core researchers who were able to synthesize structural and biochemical information from inherently complex systems into a coherent and satisfying hypothesis of bio-molecular function. Importantly, each of these hypotheses has been robust and has served to frame questions that have led to subsequent advances. They not only helped to drive forward our understanding of the molecular actors at their center stage, they also challenged us to create new tools in order to study them in greater detail. Developments in crystallography played a central role by first providing the structures of individual players and more recently the structures of the complex molecular machines that accomplish specific biological functions. The challenges presented by the complexity and dynamic nature of these molecular machines helped to build alliances among the practitioners of modern crystallography, electron microscopy, NMR, and other biophysical tools - all of which are needed to solve these giant structures.

As our tool set becomes larger and more expensive, the politics of science funding and the social aspects of collaboration have become more obviously important to progress. Science is an essentially human endeavor, and our modern day reflections on the DNA and muscle stories show that history will call out these aspects and provide windows for learning beyond our scientific hypotheses. Rosalind Franklin and Jean Hansen were strong, accomplished women scientists who made central contributions to these discoveries and they were contemporaries at King's College. They both were survived by their male colleagues. Much has been written about the environment Rosalind Franklin experienced at King's and there is controversy over whether her contributions were appropriately acknowledged when the Nobel Prize was given to Watson, Crick and Wilkins. Jean Hansen's contemporaries, collaborators and competitors alike, celebrated the 50th anniversary of the sliding filament model with a special meeting in her honor at King's. The different outcomes here reflect the differences in personalities of the players.

Individual personalities also drive the politics of science and science funding. Two areas are receiving major attention today that will help write continuing chapters in the DNA and muscle stories. The announcement of the completion of the massive Human Genome Sequencing Project was carefully staged to coincide with the 50th anniversary of the *Nature* publications about the DNA double helix. This first large scale biology project has given birth to genomics, structural genomics, proteomoics, and metabolomics initiatives that are establishing discovery science at the molecular level on a previously unimaginable scale. The promise made is that cataloguing masses of data about the molecular players in biology will lead to breakthroughs in medicine and provide the data that will

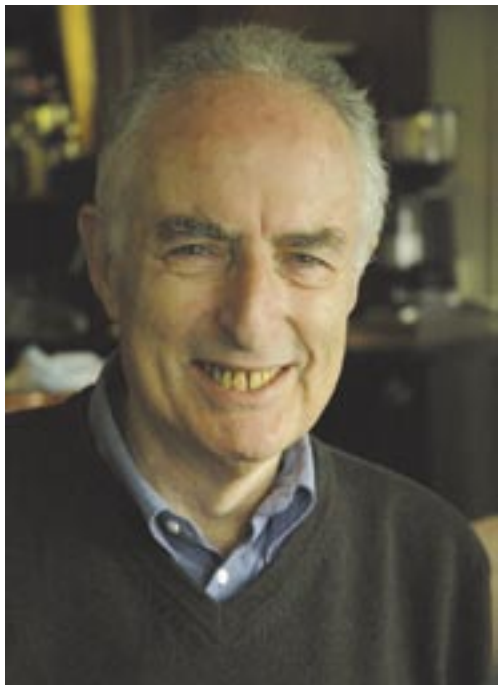
enable us to gain a predictive understanding of biology at the level of whole systems; molecular networks, cells, and even multi-cellular units. At the other end of the spectrum, we have the National Nanoscience Initiative which seeks to understand how to take individual molecules, including biological molecules or molecules that mimic their properties, to create nano-scale materials with emergent properties that can be used in a plethora of applications in biomedicine and technology development.

Both the "omics" and nanoscience revolutions hold great promise for those of us who are driven to understand how biological structures do their work. They are both developing new tools to study more and more complex systems in a quantitative way, and muscle is a quintessential nano-scale machine which still holds back the essential secret of how force is generated. The important gap in our understanding of muscle function, in spite of the fact that we have beautiful structures for the major molecular components, is the actual physical basis for force generation. Part of the mystery resides with those structures in muscle for which we have no crystal structures, such as the critically important linkage between the myosin head group and its coiled-coil tail. More basically, however, we do not know how the chemical energy released upon ATP hydrolysis by the acto-myosin complex is converted into the mechanical energy required for force generation. While there is speculation that endothermic energy is generated when the relatively flexible actin and myosin molecules form their complex and become more rigid during the contractile event, how such an entropically driven process generates the enthalpic energy required for mechanical force generation is quite unknown.

As we look to the unanswered questions that are the real drivers for structural biologists, it seems likely that the next breakthroughs may come with the new alliances that are forming between experimentalists and computational modelers. Understanding biological complexity will require computer simulations that predict behavior at multiple time and length scales. Such an accomplishment will be an epoch making breakthrough, when once again we will be witness to the creativity that can synthesize structural and biochemical information from inherently complex systems into a coherent and satisfying hypothesis. The anticipation of the next chapter in this story is inspiration for us all!

Jill Trewhella

Ewald Prize to Philip Coppens



Philip Coppens, SUNY Distinguished Professor and Henry M. Woodburn Chair of Chemistry in the University at Buffalo Department of Chemistry, will receive the Ewald Prize at the Opening Ceremony of the IUCr Congress in Florence in August.

The award, given once every three years to honor an individual who has made outstanding contributions to the science of crystallography, consists of a medal, a certificate and a cash award.

According to the IUCr citation, Philip is being recognized *"for his contributions to developing the fields of electron density determination and the crystallography of molecular excited states, and for his contributions to the education and inspiration of young crystallographers as an enthusiastic teacher by participating in and organizing many courses and workshops."*

A UB faculty member since 1968, Philip and his coworkers have played a major role in developing and maintaining the XD non-commercial software program, which applies knowledge about chemical bonds to x-ray crystallography and, conversely, extracts such knowledge from x-ray crystallographic measurements. Now being used in more than 120 laboratories worldwide, XD helps scientists more clearly define boundaries between atoms, providing a way to calculate properties of molecules and the nature of bonding between atoms, information critical to the understanding of drug-substrate interactions.

In recent work, the Coppens research group has been developing methods for time-resolved diffraction, which gives information on species that exist for very short times. The group overcame one of the field's most formidable challenges, when they captured the first structures of high-energy states of molecules that exist for just millionths of a second. Such states play a crucial role in processes such as photosynthesis. Coppens coined the word *photocrystallography* for the technique, which uses intense laser pulses timed to coincide with x-ray pulses to reveal the structure of highly reactive molecules in these transient states.

Philip was awarded the Royal Swedish Academy of Sciences' Gregori Aminoff Prize in 1996, In 1995 he was selected as the first winner of the Hauptman-Woodward Medical Research Institute's David Harker Award in recognition of his outstanding contributions to the advancement of the science of crystallography. He has also received the highest French national university honor for foreign scholars, Doctor Honoris Causa, from the University of Nancy and is a corresponding member of the Royal Dutch Academy of Sciences. He served as president of the IUCr from 1993 to 1996, and is a former president of the ACA. He received the ACA's Buerger Award in 1994. He has also served several terms as a member of the USNCCr.

Alex Wlodawer Receives Honorary Degree

The Technical University of Lodz in Poland awarded **Alexander Wlodawer,** of the Macromolecular Crystallography Laboratory at the National Cancer Institute at Frederick, MD the degree of Doctor Honoris Causa. The Technical University of Lodz, one of the largest polytechnics in Poland, has a very strong crystallographic community and counts among other honorary doctors Herbert Hauptman (1992) and William Duax (1999).

The ceremony, held in Latin, cited Alex's accomplishments, including structural studies of HIV proteins and applications of neutron and synchrotron radiation in protein crystallography. In his award lecture, Alex spoke about the contribution of protein crystallography to structure-based and target-based drug design, highlighting the most successful examples, including the development of anti-HIV drugs based on the structure of retroviral protease discovered in his laboratory. To the delight of the audience, which included a contingent of students, Alex gave his lecture in Polish! It was a homecoming for Alex because he was born in Poland and obtained his education in biophysics at the University of Warsaw. His mother, Paulina Wlodawer, is one of the pioneers of biochemistry in Poland. After the celebrations, Alex and his wife Alla Gustchina spent a memorable weekend with friends and associates.

Mariusz Jaskolski

Alex Wlodawer (left), receives diploma from Jan Krysinski, Rector Magnificus of the Technical University of Lodz. At far right: Grzegorz Bujacz, Deputy Dean of the Faculty of Biotechnology and Food Sciences, the Promoter of the award.

ACA Members - Please Check Your Directory Email Address

Almost a quarter of the email addresses in the ACA membership directory on the web have been found to be incorrect. Please check your address and send corrections to: aca@hwi.buffalo.edu.

SER-CAT Award to Nicole LaRonde-LeBlanc

Nicole LaRonde-LeBlanc received the first **SER-CAT Young Investigator Award** at the 2nd Annual SER-CAT Symposium held at St. Jude Children's Research Hospital in Memphis, Tennessee, on March 18, 2005. The award recognizes her contribution to the SER-CAT scientific program through her studies of Rio kinases. Using MAD data collected at SER-CAT, LaRonde-LeBlanc solved the structures of two unique kinases from *Archaeoglobus fulgidus,* Rio1 and Rio2. Her paper on the structure of Rio2: *Crystal Structure of A. fulgidus Rio2 Defines a New Family of Serine Protein Kinases,* was published in the September 2004 issue of *Structure*.

Nicole received her B.S. in Chemistry from Rivier College in Nashua, New Hampshire, and her Ph.D. in Biochemistry from Johns Hopkins University School of Medicine in 2002. She is currently a Postdoctoral Fellow in the Macromolecular Crystallography Laboratory at the National Cancer Institute in Frederick, MD.

The Young Investigator Award was designed to recognize an important technical or scientific accomplishment by a young investigator (within two years of his/her Ph.D. degree) at, or of benefit to, SER-CAT. The award is open to both post-doctoral and senior graduate students from any institution carrying out experimental activities at the SER-CAT facility.

SER-CAT is the acronym for Southeast Regional Collaborative Access Team, an organization consisting of 23 member institutions which was formed in 1997 to provide third generation x-ray capabilities to macromolecular crystallographers and structural biologists. SER-CAT is directed by Bi-Cheng Wang, University of Georgia, and is located at the Advanced Photon Source at Argonne National Laboratory. For more information, visit booth # 605 at the 2005 ACA Annual Meeting in Orlando, or visit **www.ser-cat.org**.

Lisa Horanyi, SER-CAT

Art in Crystallography Prize

The Editors are currently accepting entries for the new ***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.

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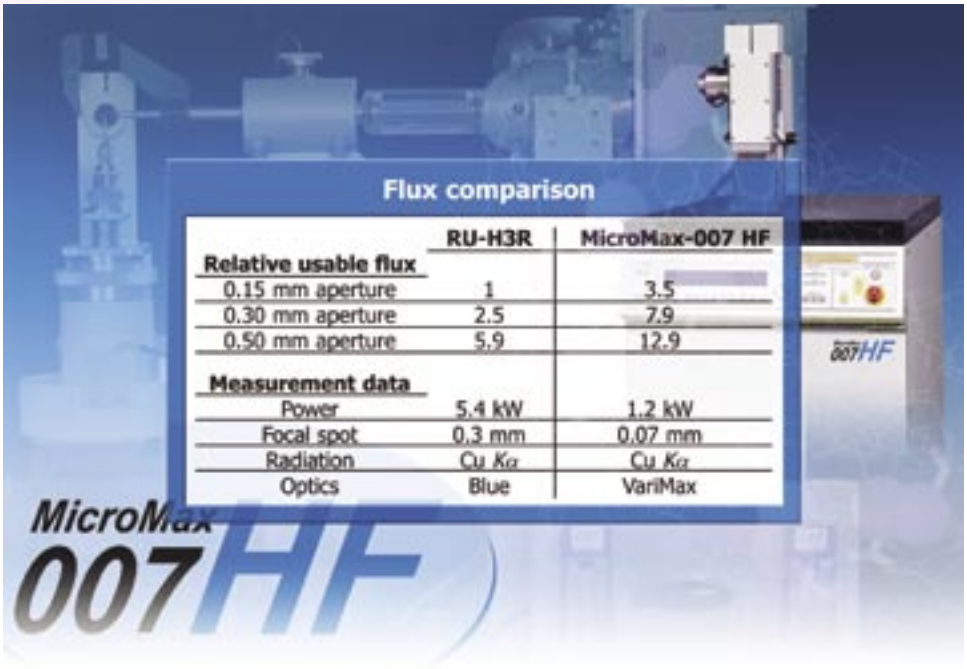

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Highlights of Fall Council Meeting

Funding Research: The ACA Council met on Sunday, November 14th, in Washington, D.C. Invited to this meeting was Ken Dill, Professor of Biophysics at UCSF and former President of the Biophysical Society, who presented council with a formal invitation for ACA to join a coalition of U.S. basic research societies in the public affairs initiative ***Bridging the Sciences***. The aim of this initiative is to establish a new federal funding institute to support basic research at the interface between the life sciences and the physical sciences. (For more information, visit **www.biophysics.org/pubaffairs/bsc.htm.**) The ***Bridging the Sciences*** coalition and the invitation to join in the initiative were discussed with the membership at the ACA business meeting held during the annual meeting in Chicago. Council concurred with the coalition in that there are compelling needs to achieve higher levels of innovation by strengthening and encouraging research at the interface between the biological sciences and the physical, chemical, mathematical, and computational sciences and by providing funds for research proposals that take more risk or rely less on predictable outcomes. Upon consideration of the financial status of the ACA, council voted to join the coalition and donate $4000 per year for two years in support of this initiative.

Council also considered an invitation from the Committee of Scientific Society Presidents (CSSP) for ACA to join in the financial support of a fellow to intern with the CSSP and assist with their efforts to promote issues relevant to scientists, including education, science budget, foreign student visas, national laboratories, and national user facilities such as synchrotron and neutron facilities. Council voted to support this effort with a one-time donation of $1000.

ACA Business: Council reviewed the financial status of the ACA. It is good policy for societies to have one year of operating expenses in reserve. The ACA is on track and close to achieving that goal. With this in mind, council reviewed and approved the budget for calendar year 2005.

The May 2005 Meeting in Orlando: The 2005 ACA meeting (May 28 – June 2) is fast approaching. The meeting will be held at the Walt Disney World Swan Hotel. There will be four workshops: ***1-Macromolecular Structure Validation, 2-Biology on the Colloid to Nanoscale, 3-Powder Diffraction, and 4-CCP4.*** The **A.L. Patterson Award** will be presented to **T. Alwyn Jones** (University of Uppsala, Sweden). The **Margaret C. Etter Early Career Award** will be presented to **Jennifer Swift** (Georgetown University). The ***Transactions*** Symposium, chaired by Anthony Kossiakoff (University of Chicago), is titled ***New Horizons in Structure-Based Drug Design.*** The full schedule, including abstracts, can be viewed on the ACA web site.

Hawaii for 2006: Council had been reviewing several sites for the 2006 ACA meeting. Much consideration was given to location, ease of travel, meeting expenses, and the expenses attendees would incur, as well as the impact that location would have on possible participants and thus the scientific program. Council voted to have the 2006 meeting in Hawaii. An ACA meeting in Hawaii presents a unique opportunity for joining with crystallographers in the eastern rim countries, as it did more than 25 years ago when the ACA last met in Hawaii. **The 2006 ACA meeting will be at the Sheraton Waikiki Beach Hotel in Honolulu, Hawaii from July 22-29.**

Lisa Keefe, ACA Secretary

PDS Election Results

The Pittsburgh Diffraction Society's annual Board of Directors elections, held in November 2004 had a hotly contested run for President-elect. The two candidates were Jennifer Aitken (Dusquesne University) and Thomas Koetzle (Argonne National Laboratory). In a very close election, Tom was voted in as President-elect. We hope that Jennifer will consent to run again. The incumbents (Bryan Craven and Charles Lake) for the two other officer positions that were available, Member-at-large and Treasurer were successful in retaining their positions with the Board. Congratulations to all of the new (and old) members of the Board of Directors of the Pittsburgh Diffraction Society.

The current Board of Directors consists of: **Alan Pinkerton** (President), **Tom Koetzle** (President-elect), **Tom Emge** (Past-president), **Bryan Craven** (Member-at-large), **Charles Lake** (Treasurer) and **Allen Oliver** (Secretary).

Further details of this election and PDS news and information can be obtained at the PDS web page, **www.pittdifsoc.org.**

Allen Oliver

Call for Nominations for Margaret Etter Early Career Award, 2006

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 2006 ACA Meeting. Please see the winter *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 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 has been extended, but please send nominations as soon as possible.

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VISA TIDE TURNING??

WASHINGTON, Feb. 13 - Responding to concerns that onerous visa requirements are discouraging foreign students and scientists from coming to the United States, the State Department has extended the time many of them can remain before renewing security clearances. The change will lengthen the validity of the clearance to up to four years for students & two for working scientists, making it easier to remain in the United States for the duration of work or study programs. Until now, they had to reapply for clearance each year.

The security clearance program, known as Visas Mantis, was established in 1998 to prevent scientists from illegally transferring technology out of the country. A study released last February by the Government Accountability Office found that scientists had been waiting an average of 67 days for a decision on their Visas Mantis clearances. The Institute of International Education found that the number of foreign students enrolled in American colleges decreased in the 2003-2004 academic year, the first decline since the 1970's.

The State Department has taken other steps to expedite Visas Mantis security clearance, including investing $1 million in technology upgrades. The agency estimates that the extension will reduce by 50 percent the number of Visas Mantis clearances to be handled each year.

"Peer Review" by Nick D. Kim, Dept. of Chemistry, University of Waikato, New Zealand. To see Nick's other cartoons, visit: http://nearingzero.net/.

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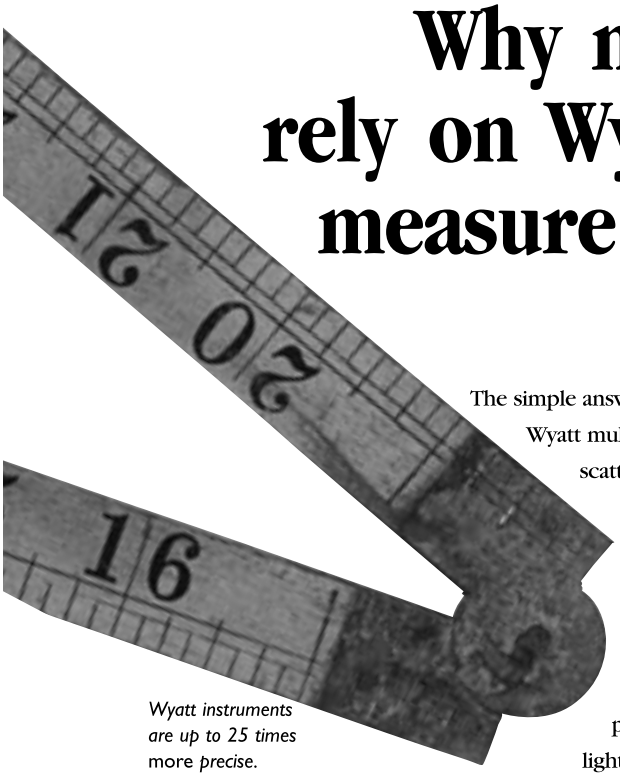

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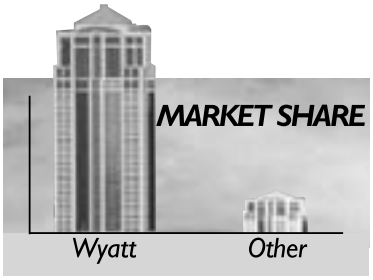

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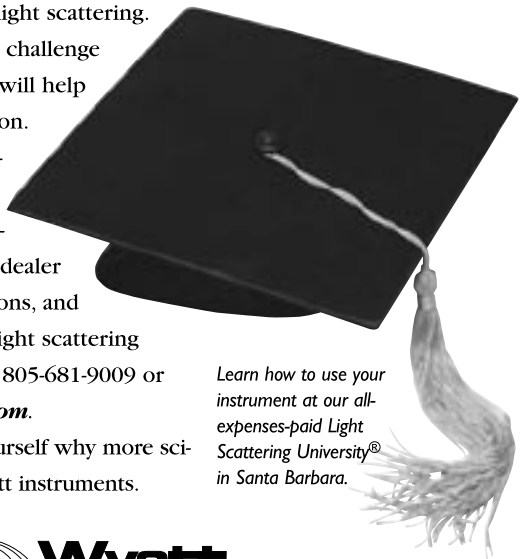

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Muttaiya Sundaralingam (1931 - 2004) and Indrani Sundaralingam (1941 - 2004)

Muttaiya Sundaralingam, 73, and his wife Indrani, 63, died together the morning of December 26, 2004 when their hotel on the beach in Nilaveli, a small village just north of Trincomalee, Sri Lanka was struck by the tsunami. The Sundaralingams were vacationing with their daughter Sharmini Shanker, and her husband, Shiva Shanker, along with their 3 children, ages 2-7. The Shanker family were not injured in the disaster because they happened to be staying at a hotel in Colombo at the time.

Muttaiya Sundaralingam, known as Sunda, was born in Taiping, Malaysia on September 21, 1931. He attended Kokuvil Hindu College (1949-1951) and the University of Ceylon-Colombo (1952-1956). In 1959, at the age of 26, he came to the United States, and three years later obtained a Ph.D. in Chemistry in the field of Crystallography with G. A. Jeffrey, University of Pittsburgh. After a postdoctoral period with Lyle H. Jensen at the University of Washington, he was appointed Research Instructor in the Department of Biological Structure there. He subsequently held positions at Harvard University, Case Western Reserve University,and Oxford University, and from 1969 to 1990, served as the Director of Biological Crystallography in the Department of Biochemistry at the University of Wisconsin-Madison. Sundaralingam joined Ohio State University in 1990 where he was named Ohio Regents Eminent Scholar and Professor in the departments of chemistry and biochemistry and Director of the Biological Macromolecular Structure Center. Sunda had recently retired, but continued his research interests as an Emeritus Professor.

Indrani Sundaralingam, also known as Indra, was born in Trincomalee, Sri Lanka on November 2, 1941. She attended St. Mary's School in Trincomalee and then Madras University. In 1966, Indra came to the United States to marry Sunda.

Sunda had an abiding interest in the stereochemistry of nucleotides and nucleic acids, the blueprint of life. This had implications for the structural principles governing the folding of nucleic acids, about which little was known at the time of his research. Based on crystallographic studies of nucleotides and molecular modeling, Professor Sundaralingam and his many students built a unified view of the structural principles dictating nucleic acid conformations. He identified the critical role played by the sugar moiety in determining the conformation of the nucleotide repeating unit and, ultimately, the sugar-phosphate backbone of nucleic acids. The principles developed have been borne out in practice time and again in subsequent work done in his laboratory and by scores of other scientists worldwide. His work is so often cited in the literature and in textbooks of biochemistry and biophysics that he was among the top 300 of the 1,000 most cited scientists for work published from 1965-1978. Among his honors are a John Simon Guggenheim Foundation Fellowship, Oxford, 1975-1976 and, in 1986, a University of Pittsburgh Alumni Distinguished Achievement Award.

Muttaiya and Indrani Sundaralingam are survived by their 3 children Sharmini, of Upper Arlington, Ohio; Rohan, of Chicago, Illinois; and Mohan, of Columbus, Ohio; and their grandchildren Nirvan, Kiran, and Sahaana Shanker. Sunda is survived by 7 brothers: Nadarajah (Singapore), Navaratnam (Malaysia), Ratnasabapathy (Malaysia), Gunaratnam (England), Darmarajah (Sri Lanka), Paramesvaran (Lancaster, CA), Kulasingam (Lancaster, CA) and one sister, Thilakavathy (Canada). Preceding him in death were another brother, Vernugopal, (New Jersey, 1933-2004) and a sister Saraswathy (Sri Lanka, 1935-1994). Indrani is survived by 5 brothers in Madison, Wisconsin: Ananda, Sivalingam, Manogaran, Baheetharan, Chandrakanthan and one sister, Sakunthalarani of Columbus, OH.

The Sundaralingam's sons, Mohan and Rohan, said: "Though the sudden and tragic loss of both of our parents by this massive, unforeseen force of nature is extremely painful for us, we can only be comforted by the thoughts that our parents perished together in the island that they knew as their homeland."

The Sundaralingams are also mourned by Sunda's many students, and by his many friends and colleagues in the crystallographic community.

Editor's note: We would be pleased to publish rememberances of the Sundaralingams and invite colleagues and former students to send them to us by May 1st, in time for the Summer *Newsletter.*

The photograph of Sunda and Indrani is from the Memorial Service in their honor, courtesy of Judith Gallucci, to whom it was given by Mohan Sundaralingam.

Dale E. Sayers, 1944 - 2004

This photo of Dale was kindly provided by Sally Ramey at North Carolina State University,

Dale E. Sayers, a founder of XAFS spectroscopy and the International XAFS Society, passed away November 25th from complications following a heart attack on Nov 9th. He was 60 years old; his wife Anne was at his side. A professor of physics at North Carolina State University, Dale earned his bachelor's degree at the University of California at Berkeley and both his master's degree and doctorate at the University of Washington. He was considered a key pioneer of XAFS technology, and was a founder of the International XAFS Society (IXS) which represents all those working on the fine structure associated with inner shell excitation (near edge and extended) by various probes (e.g. x-rays and electrons), and related techniques for which the data is interpreted on the same physical basis. Dale published the first XAFS paper in 1971, initiating this new field of research. XAFS and related spectroscopies are now a major experimental tool employed by researchers around the world. At their biennial meeting in Sweden in 2003, the IXS presented Dale with it's highest honor, the IXS Outstanding Achievement Award. Dale's work using synchrotron radiation led him into a broad variety of research topics including investigations of amorphous materials, biophysical specimens, contaminated soils, nanoscale structures, and cancerous tissues. He was a recipient of ACA's Bertram Eugene Warren Award in 1979, with F.W. Lytle and E.A. Stern for the ***Theory and Application of Fine Structure at Absorption Edge Effects***. He was also the recipient of the Case Centennial Scholar Award (Case Western Reserve University); and the N.C. State Alumni Association Outstanding Research Award. He was a Fellow of the American Physical Society.

Remembering Estela M. Roque Infante

(Manzanillo, Cuba, 1964 - Mérida, Venezuela, 1999)

In December, 1994 an Advanced Course on Single Crystal Diffraction was organized in our laboratory. Herb Hauptman, I. David Brown, Chuck Strouse, and Bill Duax came as invited speakers. With this photo Bill captured the moment when Estela was introduced to Herb and Edith Hauptman by Graciela Díaz de Delgado. The young man, Hector Novoa de Armas, from Cuba, was a visitor in the lab at the time.

Along with our ACA dues for 2005, we added a small contribution in the memory of Estela Roque Infante. Estela was a young physicist from Cuba who came to our laboratory with the hope of carrying out graduate studies in our Chemistry Department. From the beginning, she demonstrated a unique ability to carry out quality work in crystallography. Estelita (as all of us called her) besides being an excellent student and researcher, was an accomplished pianist. She graduated in piano performance and teaching in La Habana but decided to study physics. In 1987, after graduating from Universidad de Oriente in Santiago de Cuba, she started work as an Instructor in the Physics Department. With strong encouragement from her parents, family, friends, and professors (in particular from Prof. Oscar Au-Alvarez) she came to the Universidad de Los Andes, La Hechicera, Mérida, Venezuela in September of 1994 to carry out graduate studies. She had to leave her four-year old son with her parents. At the end of 1996 she obtained a M.Sc. Degree in Chemistry. Her thesis included the structural characterization of several semiconducting compounds using single crystal and powder diffraction techniques. She went back to Cuba for a short period of time and then was granted permission to continue her studies in a Ph.D. degree program. Since she wanted to get experience in other types of materials, she started to work on organic and metal-organic compounds. Estela undertook this new challenge with her characteristic enthusiasm. She completed the courses required for the Ph.D. degree and made great progress in her thesis. Unfortunately, she did not know she was suffering from Lymphangioleiomyomatosis (LAM according to the NIH-Rare diseases office). Estelita died on Labor Day, May 1, 1999, perhaps the first case of LAM seen in Mérida. She was cared for by our coworkers Rafael, Nexzy, Oleida, Asiloé, Belkis, Teresa, Alex, Jines, Auribel, Gerzon, and by many friends from our lab and our Department. It was a great loss for all of us. Estela was a hard working, very promising crystallographer who always thought she would go back to Cuba to help strengthen crystallography in her country and in Latin America. We encourage ACA members to contribute in the memory of Estela Roque Infante and/or to the ACA Latin American initiative.

Graciela Díaz de Delgado and Miguel Delgado

William B. Pearson (1921 - 2005)

Bill Pearson in May, 1995, presenting the WB Pearson Medal to Ph.D. graduate JR Devlin.

(The photo is from Chris Hughes, University of Waterloo.)

William B. Pearson died peacefully at home in Ariss, Ontario on Wednesday, February 23, 2005. Born on July 1, 1921, he emigrated to Canada with his parents in 1927. He was educated at Kingston Consolidated School in New Brunswick, at Christ's Hospital, UK and at Oxford University where he obtained first class honors in chemistry and completed his studies as a D.Phil. student with William Hume-Rothery, FRS, the legendary alloy pioneer. He served in WWII as a pilot on Ferry and Transport Commands of the RAF. Bill worked as a Research Scientist at the National Research Council of Canada (NRC) from 1952 until 1969. He then joined the faculty at the University of Waterloo where he served as Professor of Chemistry and Physics, as Dean of Science and eventually as Distinguished Professor Emeritus.

Bill was the author of several books and many scientific papers on low-temperature physics, physical metallography, Fermi surface, the chemistry of semi-conductors, and crystallography during his career at the NRC and the University of Waterloo. In addition, he edited 26 volumes of *Structure Reports* for the IUCr. He was a Fellow of the Royal Society of Canada, and held "Hume-Rothery Awards" from The Metallurgical Society of the A.I.M.E. and from the Institute of Metals in London. He was appointed a Member of the Order of Canada in 1996.

The W. B. Pearson Medal was created in his honor, and to recognize his contributions to the University of Waterloo and to Canada as a research scientist and teacher. Since 1983 five medals have been awarded annually to Ph.D. graduates, one in each of the five science departments at the University, in recognition of creative research presented in the students' theses.

Bill loved activity and hated ambition and committee meetings, and so he was a "creator of beautiful gardens, builder of many buildings, and a landowner who felt compelled to produce food." What pleased him greatly in a lifetime of opportunities he ignored because of the pressures of current interests, was the award of an honorary D.Sc. from the Royal Military College of Canada in 1984. This was based on his previous military capability and on his very visible and active participation in the Canadian Metals Physics Conferences held at RMC. since their inception in 1952.

He is survived by his wife of 38 years, Ellen Mary; his son Cedric, daughter Cecily, and their mother, Lois Jeannette Pearson of Ottawa; and his sisters Jean Stuart of Corpus Christi, Texas, and Christine Garnet of Ottawa. Respecting Bill's wishes, there will be no formal funeral service. Friends will be invited to share Bill stories in May or June when the weather is more clement.

Chung (Peter) Chieh, Chemistry Department, University of Waterloo

Contributors to This Issue:

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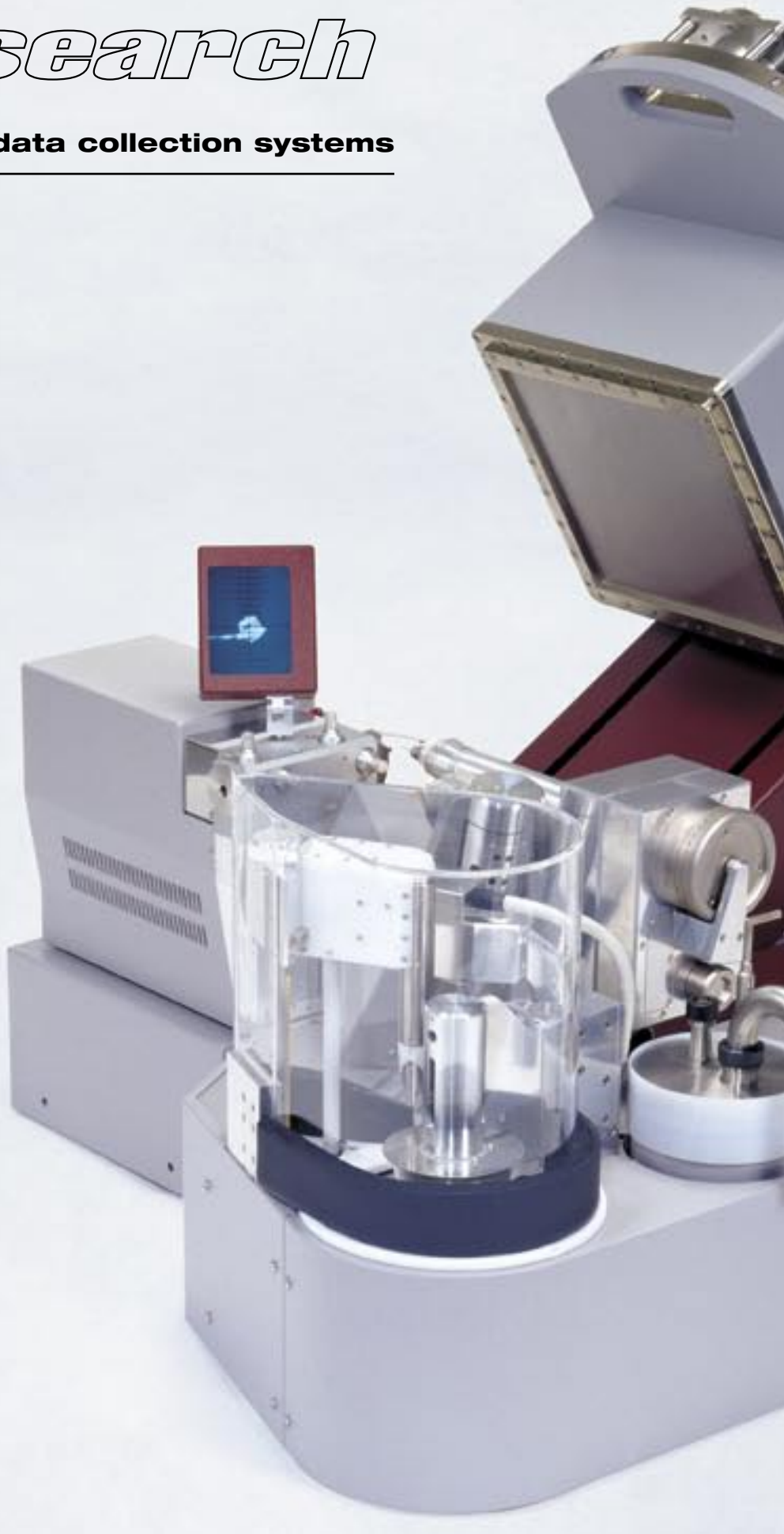

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The Cambridge Crystallographic Data Centre: www.ccdc.cam.ac.uk

40 years of database development, software and research

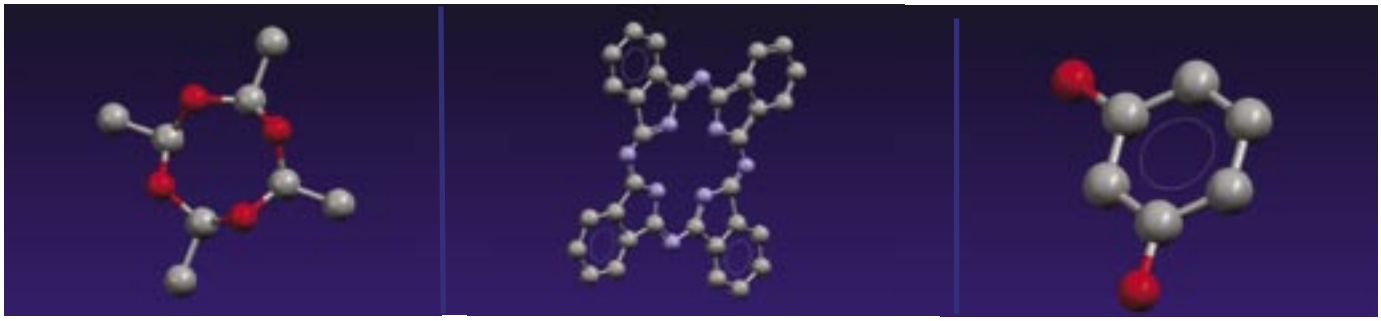
From left, former Directors David Hartley and Olga Kennard, and current Executive Director Frank Allen. *(Photograph by Dr Sarah Houlton, Chem@Cam Newsletter)*

Beginnings: The CCDC was created to record crystal structures, and the Cambridge Structural Database was one of the first numerical databases created anywhere in the world. The CCDC originated from a small group set up in 1959 by J.D. Bernal and Olga Kennard, initially at Birkbeck College, London and from 1962 at the Chemistry Department in Cambridge, collecting data on organic and metal-organic crystal structures and using these to investigate intermolecular arrangements and forces. In January 1965 David Watson joined the group and later that year the CCDC was formally established with a grant from the Office for Scientific and Technical Information. The collection of data was greatly accelerated and both numeric and bibliographic data were transferred from edge punched cards to "machine readable" form. Subsequent CSD growth statistics suggests that, had this work started later, it is doubtful if it would have started at all. But it did, and 40 years later the CSD contains 335,276 structures.

Development: By modern standards, early progress was horribly slow: computer technology was in its mainframe, card chewing, batch-processing era, and hardware was temperamental. Increasingly, other members of the research group were attracted into the new informatics world, since crystallographer-programmers were needed to turn the vision into a reality. However, they depended on effective systems for logging, organizing and encoding raw data, and scientific abstractors and data entry personnel, most of whom worked from home, were also vital early colleagues on the developing production line. The CCDC became a hub which managed a complex data preparation network, as well as a scientific analysis center that processed the raw material into a growing database. Data acquisition itself has now completed its own transformation from the days when all coordinates were printed to the current nirvana of electronic deposition via the CIF. In between we had to cope with the myriad vagaries of hard-copy depositions, which even involved some in handwritten form!

An early need was for structure validation software, to guard against local data entry mistakes and to locate the errors that occurred in some 10% of typed or typeset tables. Many errors were trivial, but in the pre-email era a significant number had to be referred back to authors by letter. Crystallographers took these "CCDC letters" in good part, and this was the beginning of a special relationship with the international community that has enhanced CSD development throughout the past 40 years.

An electronic bibliographic file was being regularly updated by 1970, and was disseminated via the Molecular Structures and Dimensions book series – itself one of the earliest handbooks to be typeset directly by computer. Meanwhile, the first 5,000 crystal structures were being validated and entered into a CSD data file. Finally, it was realised that a system of chemical structure representation was needed and a third component, a file of chemical connection tables, was created. 2D and 3D substructure search capabilities were now possible, adding tremendous value to the underlying crystal structure information. These three separate files were eventually amalgamated into the CSD that we know today.



Published in 1936, these are the three earliest structures with full 3D coordinates stored in the CSD. Metaldehyde (L. Pauling & D.C. Carpenter, JACS, 58, 1274, 1936), Phthalocyanine (J.M. Robertson, J.Chem.Soc., 1195, 1936), and Resorcinol (J.M. Robertson, Proc.Roy.Soc. Lond., Ser. A, 157, 79, 1936). No R-factors are recorded for any of these structures! The earliest references, (which do not report 3D coordinates), are from 1923: Beryllium oxypropionate (Bragg & Morgan, Proc.Roy.Soc.Lond., Ser. A, 104, 437,1923) and D-Mannitol (Backer & Rose, Z.Phys., 14, 369, 1923).

Millions of lines of code: Software development has always been at the heart of CCDC activities, and we have run the gamut from FORTRAN II to our current object-oriented C++ environment. FORTRAN, as its name implies, was never really created for text processing, and we pushed the available compilers to their limit and beyond in the early days.

The CCDC is responsible for three types of code: that which underpins CSD creation, that which forms part of the CSD System for search, analysis and structure visualization, and applications software that uses crystal structure data to solve problems in structural chemistry and biology. CCDC software developers have blended the 3D representations of crystallography with the 2D representations of chemical informatics, and have been at the forefront in creating novel systems for 3D substructure searching, including searches for intermolecular interactions, and the statistical analysis and visualization of parameter distributions retrieved from the CSD. More recently, we have generated knowledge-based libraries of structural information, and have diversified (often collaboratively) into software applications that use crystal structure information in problem solving.

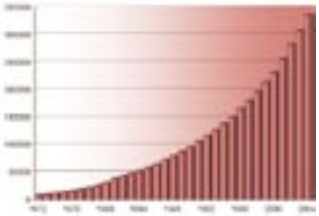
CSD System releases: By the mid-1970s, the first version of the CSD System had been released to academics in the UK, USA, Japan and Italy. In the USA, the NIH has played a key role in facilitating CSD access, both for their own research and more generally. Jim Silverton was the first customer in 1972, and the NIH has provided basic funding for CSD access since the late 1980s. Many other countries formed academic National Affiliated Centres and became subscribers to the service. The pharmaceutical and agrochemicals industries began to experiment with computational chemistry and modelling tools for rational molecular design, and the number of industrial subscribers began to rise during the 1980s.

Early releases were on magnetic tape, and the number of 1600 foot tapes per release was certainly a challenge for the average postman, particularly the one who "delivered" several CCDC parcels to a hedge "somewhere in Europe." Software was released as source code, to be compiled under the user's local operating system. Today all that has changed, with several universal operating systems, CDs and internet downloads, click-of-a-button installers, and email support desks.

1,200 Applications Papers: The first papers that made use of the CSD for fundamental research began to appear in the late 1970s, inspired by the work of Hans-Beat Bürgi and Jack Dunitz on structure correlation. Recognising the CSD as a growing library of geometric structures, there was a rapid acceleration in this type of research from about 1980. A key issue was to improve database searching and develop a proper statistical basis for data analysis, so that improvements in distributed software were often driven by current research needs.

The CCDC itself has been heavily involved in this research effort, and has published applications papers covering both intramolecular and intermolecular topics. Tables of mean bond lengths published in *J.Chem.Soc, Perkin Trans.* (1987, pp S1-S19) and *J.Chem.Soc. Dalton Trans.* (1989, ppS1-S83) have now jointly received more than 10,000 citations. In the study of intermolecular interactions, the CSD has underpinned many fundamental contributions. These have helped to provide tools for studying protein-ligand interactions, and played a part in the emergence of crystal engineering as a sub-discipline. The CCDC's most cited paper in this area – more than 1,000 citations and the 60th most cited paper ever in the first 125 years of *JACS* – is the categorization of short C-H…O interactions as true H-bonds (Taylor & Kennard, *J. Amer. Chem. Soc.,* **104,** 5063-70, 1982), work that re-shaped the global view of weaker interactions. The CCDC maintains a web-accessible database of published applications of its products, and the 1,200 current entries chart the many and varied uses of the CSD. The CCDC is well represented with over 150 papers, but more than 1,000 other references show the truly international impact of CSD-based research.

The CSD at 40: On 1 January 2005, the CSD contained 335,276 crystal structures and grew by nearly 29,000 structures in 2004. The size and complexity of structures has also increased steadily with time. The CCDC has excellent relationships with journals, and 84 titles now require electronic data deposition to the CCDC when a paper is submitted. These data enter the CSD when the paper is published, and the CCDC now maintains a growing parallel archive of more than 160,000 original CIF depositions.



Growth of the CSD 1970-2004. At this rate of growth, the CSD will record its 500,000th entry during 2009.

Current CSD statistics are available from the website, and although the CCDC encourages direct deposition of Private Communications, these statistics refer primarily to published data. The very large number of structures that languish unpublished in laboratory records is surely a matter that must be addressed in the future. Software for data processing and maintenance of both the CIF archive and the CSD are currently undergoing a major overhaul, and new software will incorporate expert knowledge that has been gained over the past 40 years.

New Products: Two new components of the distributed CSD System have been added since 1997. These are knowledge-based libraries of intramolecular geometry (Mogul) and intermolecular interactions (IsoStar). They provide click-of-a-button access to millions of individual pieces of geometrical and chemical information that can be derived from the CSD (and PDB protein-ligand complexes in the case of IsoStar). Further development, and integration of this structural knowledge with other software, is ongoing in both cases.

IsoStar scatterplot of the distribution of O-H (donor) contact groups around ester central groups in the CSD.

Recent years have also seen the CCDC diversify into develop-

ing and marketing specific software applications for rational drug design (GOLD, SuperStar, Relibase+) and for structure solution from powder diffraction data (DASH). All of these products make use of crystal structure data from the CSD or PDB in some way, and all except SuperStar are being developed through collaborations with industry and academia. The life sciences products, concentrating essentially on protein-ligand interactions and protein-ligand docking, help to solve difficult problems, and promote the value of small-molecule crystal structure data in structural biology and in the pharmaceutical and agrochemicals industries. The CCDC continues to broaden its horizons, by seeking new areas of science in which crystal structure data adds value to research and development activities.

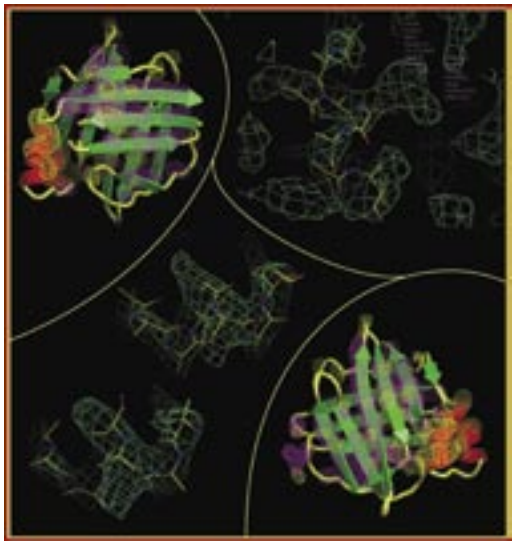
The CCDC as an Independent Institution: The CCDC was grant-funded from 1965 until 1989, when it became an independent institution: a non-profit charitable Company Limited by Guarantee under English law. This means that the CCDC must be financially self-sufficient, and that any surplus income must be used by the company (*e.g.* for new equipment) or specific charitable activities. Principal contributions here have ensured access to the CSD system in developing countries, and provided support for students and professional organizations. The CCDC's affairs are overseen by an international Board of Governors, eight eminent scientists who, in their turn, are responsible to UK Companies House and to the Charity Commissioners for England and Wales.

Our most valuable assets - staff and customers: The CCDC has expanded steadily, and now has 50 employees divided between database creation, product development, research, scientific and technical support, and administration. The CCDC now has customers in academia and industry all over the world, and the nearly 2,000 CSD System licenses were distributed across 56 countries in 2004. The CCDC has a long history of scientific collaboration with academia and industry, and this work has fueled our research output and fed into our product developments. Currently, the Pfizer Institute for Pharmaceuticals Materials Science, a major partnership involving the CCDC, Cambridge University and Pfizer Inc., is generating exciting results and further extending our areas of scientific interest.

We do not have a precise total of the number of staff and visitors who have worked at the CCDC over the past 40 years, but it must be 250 or more. What we do know is that they have left, or are leaving, their own mark on the organization. It is the stronger for their contributions. Customers, scientific collaborators and data depositors also leave their mark, through their constructive input and feedback on our efforts. The CSD, our products, and ultimately all of our customers, have benefited enormously from these interactions, and we are grateful for their involvement.

We look forward to the next 40 years.

Frank Allen



Images from Patterson Award Winner Alwyn Jones

Alwyn Jones will present the Patterson Award Lecture at the **A.L. Patterson Symposium** to be held at the Orlando ACA Meeting May 28th - June 2nd.

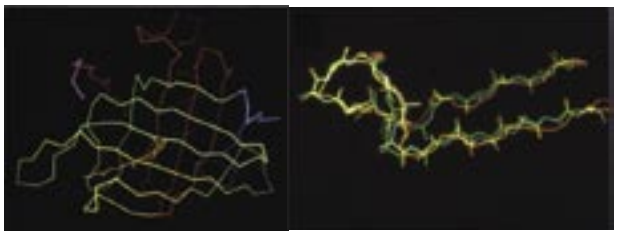
Upper left and lower right: Two views of ESSENS maps of averaged P2 myelin experimental density. Yellow contours indicate the α-helix template map and purple contours indicate the map generated using a β-strand template. All helices and strands in the three-dimensional structure are apparent, even the more distorted fifth strand of the barrel.

Upper right: A nine-residue α-helix built into the unaveraged P2 myelin experimental map at skeleton atom 710. The SST (secondary-structure template) menu is expanded and visible at right of center.

In the **center image,** a nine-residue helix was fitted to the experimental P2 myelin density with the SST system. Local averaging then verified that the directionality is correct because the C^{β} of the central residue obviously fits. In the image at **lower left,** the helix was flipped, RS fitted and the density locally averaged. This directionality is wrong as indicated by the poor fit of the same C^{β}.

The images are from Alwyn's recent paper ***Interactive electron-density map interpretation: from INTER to O,*** T. Alwyn Jones, *Acta Cryst*. (2004) **D60,** 2115 -2125. All are from the ***O*** generation of his programs. The test data for P2 myelin protein, a low resolution structure (incomplete 2.8 Å data) with three molecules in the asymmetric unit, is from S.W. Cowan, M.E. Newcomer & T.A. Jones, *J. Mol. Biol*. (1993), **230,** 1225-1246. The ESSENS template convolution method is described in G.J. Kleywegt & T.A. Jones *Acta Cryst*. (1997) **D53,** 179-185.

Editor's note: For readers nostalgic about FRODO, the images at right are also from Alwyn's 2004 paper in Acta Cryst. They are Evans & Sutherland PS330 illustrations of retinol-binding protein (M.E. Newcomer, T.A.Jones, J Aqvist, J. Sundelin, U. Eriksson, L. Rask, & P.A. Peterson (1984), EMBO J 3, 1451-1454). The near right image shows rainbow ramping (atoms colored according to position in the sequence); the image at far right shows an overlay of a traced portion of the skeleton with a polyalanine built using pentapeptide fragments from a main-chain database.



AAAS Preliminary Analysis of 2006 Federal R&D Budget

On February 7, President Bush released his proposed budget for fiscal year (2006). Against the background of record-breaking federal budget deficits, a continuing and costly war in Iraq, and expensive proposals to introduce private accounts for Social Security in the future, the federal investment in R&D would increase only modestly in 2006, with cuts far outnumbering increases.

The AAAS Preliminary Analysis of the FY 2006 budget, (see **www.aaas.org/spp/rd/prel06p.htm** or **www.aaas.org/spp/rd/prel06p.pdf),** shows that the proposed federal R&D portfolio of $132.3 billion would be 0.6 percent or $733 million above this year's funding level, far short of the 2.0% increase needed to keep pace with expected inflation. Increases for the continuing priorities of homeland security and space exploration R&D would be greater than the overall increase, leaving all other R&D programs collectively with less money next year than this year. ***Some highlights:***

- The nondefense R&D investment would increase 0.7% to $57.1 billion. While NASA would continue to receive additional resources, most other nondefense R&D funding agencies would see their funding decline or fall well short of inflation. NSF would receive an average 1% boost for research programs. The NIH R&D investment would fail to keep pace with inflation for the first time in 24 years, with nearly all the institutes receiving increases of 0.5% or less. The DOE's Office of Science would see its budget fall 4%, and environmental R&D programs would decline across the board. Multi-agency initiatives in nanotechnology, IT, and climate change science would all decline in funding.

- For the first time in a decade, defense R&D would barely increase. There would be a 21% cut to DOD's S&T investments. There would be tough choices even in agencies with increasing budgets. At NASA, a 5% boost in R&D funding would still require steep cuts in aeronautics and earth science funding and the cancellation of a proposed Hubble servicing mission to pay for NASA's ambitious space exploration plans. Although DOE's energy R&D would climb 11% because of increased investments in hydrogen, nuclear energy, fuel cells, and coal, DOE would eliminate R&D on gas and oil technologies and sharply reduce funding for some renewable energy R&D. The budget proposes to boost intramural R&D at NIST by 10%, but also proposes to eliminate NIST's Advanced Technology Program and halve the budget of the Manufacturing Extension Partnership.

- Total homeland security-related R&D, however, would jump 10.7% to $4.6 billion; within the total, the Department of Homeland Security would boost its R&D investments by 24% to $1.5 billion.

X-ray Diffraction Through the Years: from one One Structure per Year to One Structure per Hour

(from the Kenneth N. Trueblood Award Lecture by Richard E. Marsh, Senior Research Associate in Chemistry, Caltech)

Dick and Helen Marsh

This story begins 55 years ago, in the fall of 1949. I was beginning my last year of graduate work at UCLA, and a new faculty member had joined the chemistry department. It was Ken Trueblood. He had just come from Caltech, where he had received his PhD in Organic Chemistry and had stayed on for a couple of more years to work on crystal structures of amino acids. Ken brought two things that were particularly important to me. First, he brought a whole cabinet-full of IBM cards, which could be used on tabulating machines to carry out summations for Fourier calculations. (Actually, I didn't use these cards very much, as the process of picking out the correct cards was so damaging to the quicks on my finger-nails that I soon reverted to traditional methods of adding.) The second thing that Ken brought was knowledge of Caltech. In 1950 I received an offer for a post-doc position at Caltech, but was worried that it would be a too high-powered, or whatever, place for me. Ken assured me otherwise, and I've been at Caltech ever since.

1949 was the year in which the ACA was formed; its first meeting was at Pennsylvania State University in April, 1950. The IUCr had been formed in 1947, and Volume 2 of *Acta Crystallographica* was published in 1949. The basic procedures of crystal-structure analysis were understood: the Patterson function was widely used, a few simple structures had been solved (by hand) using direct phasing methods, and the application of least-squares refinement had been described way back in 1941, by Eddie Hughes. But all of these procedures were difficult, because of the computations that were needed. Punched-card machines were slowly making their way from accounting departments to crystallography laboratories, but in many laboratories nothing was available except slide rules, trigonometric tables, and mechanical calculators which were fine for addition and subtraction but iffy, at best, for multiplication and almost totally useless for division. A two-dimensional Fourier summation involving perhaps 100 terms was probably a full-day job; calculating structure factors for these 100 terms might take a week.

But times were beginning to change. Just prior to the 1950 ACA meeting, a special conference on "computers and the phase problem" was held at Penn State and organized by Ray Pepinsky. It was attended by many of the international luminaries of crystallography, and there were talks on various methods of adapting punched-card machines to expedite structure-factor and Fourier calculations. A highlight of the conference was the demonstration, by Pepinsky, of ***XRAC***, an analog machine he had designed consisting of dozens of sine-wave generators whose amplitudes and frequencies could be adjusted and combined onto a cathode-ray tube to produce, instantaneously, a two-dimensional Fourier summation; usually a Patterson summation, but adjusting the phases of the generators allowed the user to produce electron density maps as well (with the signs of the "reflections" assigned by trial-and-error).

Progress in computer development was rapid during the 1950s. A red-letter day in 1954 was the installation, at UCLA, of the high-speed computer ***SWAC***, developed by the National Bureau of Standards; it was soon programmed by Ken Trueblood and his students, including Bob Sparks, to carry out Fourier, structure-factor and least-squares calculations. On it, a structure factor could be calculated in a couple of seconds. We all know of Ken's association with Dorothy Hodgkin in determining the structure of vitamin B-12, with structure factors and Fourier maps calculated on ***SWAC***, the results mailed to Oxford, and a new set of coordinates mailed back to UCLA for another cycle.

However, in many laboratories calculations remained onerous. I recently came across, in my office, a large laboratory notebook dated 1956, kept by a very young post-doctoral associate of the time. The first 16 pages are filled with the detailed calculations necessary to convert the intensities of about 700 reflections to coefficients appropriate for a sharpened, origin-removed Patterson map; on the subsequent page, dated a month later, is the notation that she was now ready to begin the Fourier summations. I wonder if that post-doctoral associate, Jenny Glusker, remembers that month.

L to r: Ken Hardcastle, Jenny Glusker, Dick Marsh and Larry Henling. The T-shirts were done by Larry and Diana St. James with help from Ken, Cora MacBeth and Barbara Hsu.

What sorts of crystallographic errors arose in those early days? Of course, countless mistakes, usually rather trivial and forever un-noted, were made in transcription, slide-rule manipulations, and calculator operations. More serious and obvious errors were usually noted during the process of the investigation; after all, there was plenty of time for careful consideration since it often took a year or more to complete a structure. Nevertheless, some serious mistakes were made. A major difficulty sometimes arose in assembling projections down two or three different crystallographic axes (the usual procedure) into a correct 3-dimensional structure; according to my memory, a particularly knotty problem was that of deciding whether the origin chosen for a b-axis projection in space group $P2_1/c$ was the true center of symmetry or the projection of the screw axis. An example of this sort of error arose in the original description of one of the monoclinic forms of elementary selenium, where the eight-membered ring of selenium atoms contained one very short (2.21 Å) and one very long (3.04 Å) Se-Se bond, suggesting some sort of peculiar ionic structure. When the correct origin was figured out, the ring became entirely regular.

Since the 1950s, the evolution of computers has been continual and, to me at least, mind-boggling. Today, the full beauty of direct methods is at our disposal, and least-squares refinements may take less than a second rather than weeks. A complete "small-molecule" structure solution and refinement can be done in minutes rather than months. With the availability of

tremendously rapid computers and tremendously powerful programs for structure determination and refinement, there seems to be little need and, perhaps, too little time for careful consideration. I see this as something of a problem.

Approximately one year ago, Ton Spek, using a modified version of PLATON, carried out a complete survey of the Cambridge Structural Database, searching for structures that might have crystallographic symmetry higher than that reported by the original authors; he came up with something over 5000 hits. Of these, nearly 3000 refer to structures that were originally described in space group P1. I have been examining these 3000 with some care. A large number of them describe molecules that are clearly chiral with Z = 2, the two molecules being related by an approximate but, of course, inexact center of inversion. (Is there a possibility that, in other cases, such structures have been refined in space group P1-bar and described as racemic mixtures, perhaps disordered, rather than as chirally pure? (Frank Fronczek discussed this problem in his talk later in the symposium.) Many others of these 3000 structures have already been revised to higher-symmetry space groups, or have only approximate symmetry. But I believe that there remain something like 150 entries that are clearly incorrect and, as yet, un-noted. In most of these cases the correct space group is P1-bar; that is, a center of inversion, either relating two (or more) achiral molecules in the unit cell or contained within a single molecule (Z = 1), has been overlooked.

As an example of what usually occurs in situations where a center of inversion has gone un-noticed during a structure refinement, I cite a compound containing a cyclohexane ring. In the original description in P1, the C--C bond lengths appear, quite ridiculously, to range from 1.20 Å to 1.82 Å; when the structure is described in P1-bar, that is when the atom coordinates are averaged across the (unnoticed) center of inversion, the distances are entirely satisfactory: from 1.51 to 1.54 Å. Apparent distortions of this magnitude are by no means unusual; that they go unnoticed (or, at least, unexplained) by the original investigators is, to me, disturbing.

Let me point out a few other disturbing features that I often encounter in surveying structural details (CIF's, usually) of recent investigations. At the very top of my list of questionable practices is the apparent compulsion that the final "goodness-of-fit" be close to, or below 1.0. This is done by including, in the final refinement cycles, an additional parameter or two adjusting the weighting function (and, hence, the sum-of-squares of the weighted residuals) so as to create the desired value. This is, at the very best, a misleading practice. The "goodness-of-fit" should be just that: a measure of how well the derived model of the structure fits the observed data, including the experimental errors in the measured intensities. (I believe that Jim Ibers named it "the standard deviation of an observation with unit weight".) Modifying the experimental errors so as to attain a preconceived value for the "goodness-of-fit" seems indefensible. It has often been pointed out that adjusting the weights during early refinement stages may hasten convergence, but it seems to me that, in reporting the final results of a refinement, the investigator should also report an objective and unaltered measurement of how well these final results explain the original observations.

The "Flack parameter," a measure of the chiral purity of crystal, is often misunderstood and misused; it has been the focus of much discussion within the crystallographic community and should be treated with respect. The values of the final parameter shifts, in relation to their standard deviations, should be examined more carefully than they often seem to be. If these final shifts remain significant during the final refinement cycles, it is clear that satisfactory convergence has not been attained, perhaps because a center of inversion has gone unnoticed and large correlations between parameters remain. Similarly, constraining or restraining geometric quantities such as bond lengths or angles in order to create apparent convergence is a dangerous practice; there is always a danger in assuming that a preconceived structure is correct. As in other scientific experiments, it is the purpose of crystal-structure analyses to discover the correct structure, ***not*** to constrain an assumed one to be correct.

But despite the problems that I find in many reported crystal structures - problems due, I believe, to undue haste and to a conviction that the computer routines will automatically produce the correct result - crystallography remains a wonderful technique. For small-molecule compounds (and conveniently overlooking the miserable problems associated with, for example, disordered solvents of crystallization), x-ray diffraction provides a conclusive and highly precise description of molecular structures. As Frank Herbstein once said, it is "the court of last resort." A graduate student once described to me the thrill he got upon solving a structure, noting that he was the very first person in all the world to know, with absolute certainty, exactly how the atoms were arranged in that particular compound. I hope and trust that that feeling of exhilaration will continue to be felt by all of you, and that you can always take pride in knowing that the structures you solve represent a correct and highly precise piece of information that was previously unknown.

Dick, Judy Schomaker, Jack Dunitz, Bill Sly, Helen Marsh, Barbara Dunitz, & Verner Schomaker at the Marsh home in San Marino CA.

In closing, I should like to express my deep appreciation to four special people: to Larry Henling, my guru who leads me through the daily problems of coping with the modern crystallographic world; to Ton Spek, who has been of continuing help in examining structures within the Cambridge Database; to Frank Herbstein, who has been a faithful cohort during many years of examining problem structures; and to Verner Schomaker, who for many years made available to me (to do with as I saw fit!) so much of his great wisdom and insight. I am absolutely certain that Ken Trueblood would have wished to join me in a tribute to Verner.

Dick Marsh

Advanced Area Detectors for Protein Crystallography and Electron Microscopy - or: Confessions of a Reformed Physicist, by Supper Award recipient Nguyen-Huu Xuong

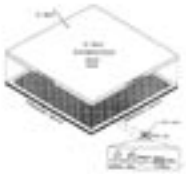
First I would like to thank the ACA President and Council members for giving me this award. I hope that you don't change your minds after hearing my confessions. I was called a reformed physicist by my colleagues due to my early training in high energy experimental particle physics. However I saw the light and made a drastic change in 1968. Looking at my *c.v.,* you would think that I moved to protein crystallography because I knew about its importance and its bright future - so my first confession is that: ***I was doing the right thing (getting into protein crystallography) for the wrong reasons.*** At that time I was using the computer to analyze the particle tracks and interactions that were imprinted on the bubble chamber films. So, my main reason to get into protein crystallography was that I could still do more or less the same thing with x-ray film. The following is an account of the methodological and instrumental side of my work after this fatalistic switch.

Prehistoric time: precession camera and screenless precession method (1968-70) Not many young protein crystallographers know about the precession camera but it was widely used in the 1950s and 1960s to collect data. One usually used a screen to select only one layer, making it easy to index the reflections. However, the screen eliminated 90% of the diffraction pattern, making the exposure time extremely long (12-24 hr) and requiring too many crystals. One day, my illustrious colleague at UCSD, Joe Kraut, suggested to me to throw away the screen. He told me that, being a physicist, I should be able to write a program to index the reflections and automatically estimate their intensities. Accepting his challenge, I first designed, together with a small company (TechOps), a rotating drum film digitizer that would accept the precession camera film. Then I wrote a series of programs to index the reflections and estimate their intensities.[1] I was more than a little amazed that the method really worked and we were able to collect a set of data which together with some diffractometer data allowed us to solve the structure of chymotrypsinogen to 2.5Å.[2] However, the screen-less precession camera method had a serious drawback. Too many reflections near a layer edge have to be thrown away due to the uncertainty in estimating their Lorentz factors, which can become very large. So it was soon replaced by the rotation camera method.[3] In the meantime, I was looking for a way to eliminate film altogether since it was inefficient in detecting x-rays and required manual handling in the development and digitizing steps.

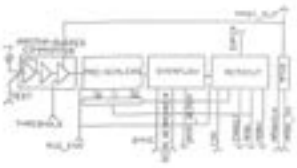
Multiwire area detector (1970-1995) I was introduced to the multiwire proportional chamber by another of my colleagues at UCSD, Prof. Wayne Vernon, also an experimental particle physicist. He helped me to adapt this instrument to protein crystallography. It was called a multiwire area detector since it was the first one to detect digitally a large area of the diffraction pattern containing hundreds of reflections (instead of each reflection individually as in the standard diffractometer). However, we would not have been successful without the arrival of a new graduate student, Ron Hamlin. Ron worked so hard to overcome the many difficulties. He was also very careful and particular in everything he did; so not only did he make the detector work, but it also worked reliably.[4] (My second confession: ***the ACA gave the award to the wrong person***.) I concentrated on the software which was simply an extension of the "screen-less precession" software. My software was hard to use. Fortunately, it was very much improved by Chris Nielson and Andy Howard.[5] Since the multiwire area detector collected data in real time, we were able to use the slice rotation method where the stepping angle is only about 0.1 degree per frame (instead of 1 degree for a standard rotation method). This method required more complex software but yielded a better measurement precision. With its speed and the precision of its data, the multiwire area detector was an instant success and, with funding from NIH, we were able to set up a research resource at UCSD where protein crystallographers came from all over the world to collect data. However, this detector also had many drawbacks: low spatial resolution (only 150 x 300 of 2 x 1 mm pixels), large spot size (6mm by 6mm), and low counting rate (about 50,000 counts per second); so after a while, it was replaced by more advanced types of detectors like the image plate scanner and the CCD based detector.

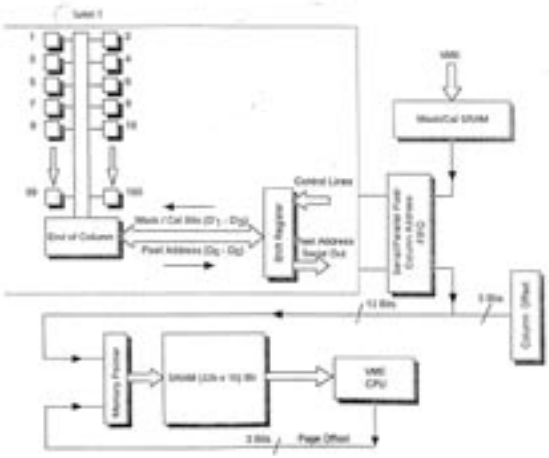
Silicon pixel array detector (1995-present) While the CCD based camera is an excellent detector, it still has inherent drawbacks. One drawback is the need to use a scintillator to transform x-rays into light. (CCDs are allergic to direct x-ray exposure.) This conversion drastically reduced the signal making the signal-to-noise (S/N) ratio of detecting a single x-ray photon about 1/1. With a direct detection detector like the pixel array detector which uses a silicon sensor, one can get an S/N ratio larger than 10/1. With this S/N ratio one can even do photon counting. In 1995, we collaborated with a group at Lawrence Berkeley National Laboratory (LBNL) to design this type of detector.[6] Once finished, this detector will be an assembly of modules of "50 x 50 pixel" arrays assembled in a tile arrangement. The detector for each module is a reverse biased Si diode array bump-bonded to an Application Specific Integrated Circuit (ASIC). The detector pixel pitch is 150 μm. The ASIC contains both analog and digital circuitry which processes a photon hit and generates the associated pixel address in less than 80 ns. Each pixel processor has a preamplifier, shaper differential discriminator and a 3-bit pre-scaler that divides the pixel event rate by 8 hence reducing the external data flow bandwidth requirements. At the end of the acquisition cycle the pre-scaler contents can be read out and combined with histogram data. An overflow bit or pseudo 4-bit starts the readout logic sequence to generate the pixel address. The event driven address is generated by the column architecture. The pixel address is then sent off chip for processing by a VME pixel module which assigns additional column and chip address encoding bits and pipes the data to the VME histogram memory processing module. The histogram data is stored in VME memory where it can be read by the CPU for processing. It should be noted that this detector

is a true digital photon counting device and offers a truly frameless read out for high speed data collection.

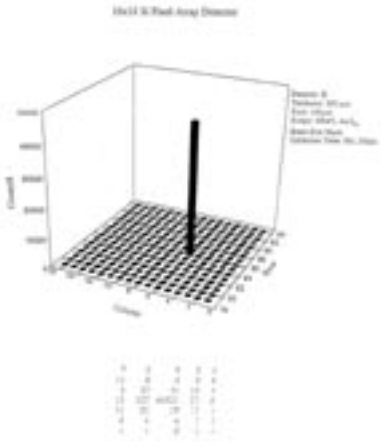


At right is a schematic diagram of the pixel array detector module showing the silicon sensor ASIC readout chip hybrid model and processing electronics. The single 50 x 50 module shown will be assembled into a larger array. The "dual column" readout diagram used in the UCSD-LBNL pixel array detector is shown below. For more information please see reference 6.





We have been able to assemble a 16 x 16 pixel array module. The figure below shows its output when illuminated with a very well focused x-ray beam. The displayed numbers of interest, centered at the peak and neighboring pixel values, clearly show the full width at 1/100 maximum is less than one pixel width.



However, we have found the "column readout" method to be too noisy since both the recording and readout are being done at the same time. Another type of photon counting pixel array detector has been developed at CERN, adapted to protein crystallography and built at the Swiss Light Source (SLS). In this detector, the photon count in each pixel is stored in a fast counter. This count will be read out only at the end of a frame. The SLS group has built a larger detector and research with it was reported in the Supper Symposium by C. Broennimann. In addition to the photon counting pixel array detector, there is the analog pixel array detector developed by the Gruner group at Cornell. In this detector, the electronic charges produced by the x-ray photons in each pixel are stored in a capacitor and will be read out through an analog-to-digital converter (ADC) at the end of each frame. This type of device is simpler to make but suffers from a too low dynamic range.

To increase the dynamic range, the collaboration between Cornell and a private company (Area Detector Systems Corporation, ADSC) is developing a modified device in which the changes produced by the x-ray photon in each pixel will be used to fill up a bucket. When each bucket reaches a predetermined level, it will be emptied. At the end of a frame, the number of emptied buckets together with the measurement of the charge left in each bucket will be sent out to the computer. This new method, called mixed mode (digital and analog) will allow a very large dynamic range (about 107:1).[7]

Detectors for cryo-EM (1998-present) I have now reached my last confession: ***Being a protein crystallographer but dreaming of cryo-EM.*** Lately, cryo-electron microscopy (cryo-EM) has emerged as a powerful method to determine the 3D structure of large protein complexes and viruses.[8] In the near future, it could rival protein crystallography. The advantage of cryo-EM over protein crystallography is that it does not depend on growing large crystals, a very time consuming and, in many cases, impossible task. The main drawback of cryo-EM is the low resolution of the structures obtainable at this time. For a virus, the best structure from cryo-EM is now 7.4Å and for a large protein complex like the ribosome, the best resolution is 11.5Å.

Cryo-EM would be much more useful if it could easily yield higher resolution structures (down to 3Å resolution). One limitation to the resolution of the structures obtained with cryo-EM is the difficulty associated with the collection and processing of the very large data sets (estimated to be up to one million images for 3Å resolution) required for statistical analysis. This difficulty arises from the necessity, in many cases, to use film to record EM images. While film provides excellent modulation transfer functions (MTF), compared to commercial CCD cameras, it requires several post-acquisition steps such as development and digitization that are cumbersome and time-consuming. Moreover, film lacks the linear response afforded by CCD camera systems.

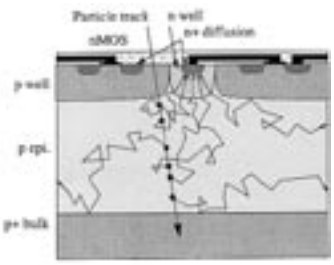
A standard detector option commonly used instead of film is the direct digital readout, charged coupled device (CCD). CCD detectors for electron microscopy are available with formats up to 4096 x 4096 pixels, although few, if any, commercial detectors deliver the full resolution of the device. First of all, for electron microscopy applications, a phosphorescent scintillation screen is needed to convert the electron image to a photonic image within a spectral range where the detector quantum efficiency is maximized.

Unfortunately, the scintillation screen not only drastically reduces the signal to noise ratio of the detector but also introduces a large spot size (up to 30 μm) for each detected electron.

Clearly, there is an urgent need for a system that would directly and automatically detect electrons. We have focused our attention on the Active Pixel Sensor (APS), which has just been invented to detect charged particles, but has never been considered before for electron

microscopy.[9] Due to its simple design and its monolithic nature, the APS can be made with a large number (4000 x 4000) of small pixels (5 μm x 5 μm). The sensitive depth region can be made as small as 8 μm, yielding a very good signal (about 1000 generated electron-hole pairs for 200 - 300 keV incident electrons) while keeping the lateral scattering of these incident electrons to a minimum of 1 to 2 μm. Therefore it can be made into an ideal detector for electron microscopy with both high resolution and high signal to noise ratio.

In order to get some preliminary results, we have used a monolithic APS being developed for charged particle tracking and imaging.[9] It has a sensitive p- epitaxial layer (about 8 to 10 μm thick) between a p-well layer and a p++ substrate. The figure at left shows a cross section of an APS with traces of ionization electrons produced by a high energy incident electron. Inside each pixel are diodes formed by the interface of an n+ diffusion and a p- epitaxial region that will collect the electrons generated by an incident high energy electron in its passage through the p- epitaxial layer. For cryo-EM, an incident electron of 200 or 300 keV will generate about 1000 electrons in the silicon which is significantly higher than the noise, typically less than 45 electrons. These generated electrons are confined in the epitaxial region until they diffuse toward one or more sensor diodes, where they are collected. Each pixel integrates the collected electrons during an exposure period. At the conclusion of the frame, the contents of the sensor array are then read out, digitized and stored. All of the integration and read out electronics are implemented near the top surface of a chip fabricated using a 0.25 μm CMOS process, and are transparent to the incident electrons. The "fill factor," *i.e.* the proportion of each pixel area that is sensitive to the incident electrons, is 100% due to the fact that the sensitive p- epitaxial layer lies beneath the readout circuitry and is continuous.

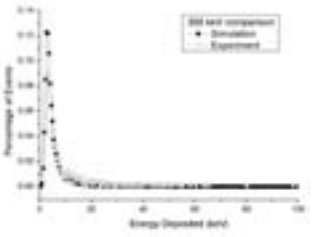


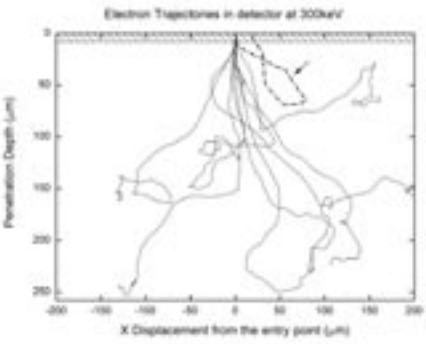
The APS used in this study, was designed by Stuart Kleinfelder at UC Irvine for nuclear physics experiments. This 128 x 128 pixel chip has a pixel pitch of 20 x 20 μm and is organized into 4 different quadrants of 64 x 64 pixels, of which one quadrant, with 4 small (1 μm x 1 μm) photodiodes per pixel, was of particular interest. The chip was designed in a standard TSMC digital 0.25 μm CMOS process that includes an 8-10 μm epitaxial layer. The analog output of the APS was digitized at 0.4 MHz to 16 bits. This chip is specially designed for nuclear physics experiments that need to detect single electrons in very short exposure frames. The exposure time of each frame was the time it took to read out two quadrants, about 20 msec. We used the correlated double sampling method to reduce reset noise by subtracting subsequent frames. As the chip was not reset between reads, the difference is simply the integrated charge in the diode during the last frame and reset noise is substantially reduced. All data were taken at room temperature.

At first we collected a thousand frames without any incident beam. A histogram of the reading of all pixels in these frames yields an average noise sigma of 1.5 ADC units. We also notice that there are very few (less than 0.1 %) readings equal to or above 25 ADC units. Therefore, a noise floor value of 25 ADC units was used as the threshold value of the detection of an incident electron or x-ray.

We have found that the quadrant with 4 small photodiodes per pixel has very good charge collection efficiency with 100% of the deposited charge collected within a 3 x 3 pixel area. For this study, we define an electron (or x-ray) event as a cluster of connecting pixels with the maximum read out at or above 25 ADC units. The energy deposition of this hit is proportional to the sum of ADC values in the area of 3 x 3 pixels centered on the maximum pixel with the maximum read-out. In order to convert the energy deposited in the detector from the pixel ADC values, we have illuminated the detector with 5.9 keV x-rays from a Fe55 source and plotted the histogram distribution of the energy deposited by Fe55 x-rays. This histogram fits a Gaussian distribution very well with a mean at 65.9 ADC units, therefore yielding a relation of 11.1 ADC units per keV of energy deposited by a particle inside the detector.

The figure at right shows the histogram of the energies deposited in the sensor by incident electrons of 300 keV where about 1800 events were counted. As expected, we see in the histogram a Landau distribution below 10 keV with a peak around 5 keV. However, many events have unexpectedly higher absorbed energy values. These events are very probably not from x-rays generated inside the EM, since the thin (8-10 μm) epitaxial layer of the detector has a very low efficiency to detect x-rays, specifically the ones above 20 keV. After careful study, we have concluded that these events are caused by incident electrons that are backscattered in the silicon substrate (250 μm thick) and re-enter the sensitive epitaxial layer a second time with much lower velocity and therefore deposit more energy into the detector. This conclusion is supported by extensive simulation experiments where we found that at an incident electron energy between 200 and 400 keV, an average of 1 out of 10 incident electrons will go through this backscattering process and re-enter the sensitive epitaxial layer a second time. One such example is the simulation of electron trajectories showing back-scattering which is illustrated at right. From the simulations, we were able to produce distributions that agree with the experimental data. This was true especially when we compared data from higher energy deposited events. Since the backscattered electrons will deposit too much extra energy in the APS (sometimes up to 20 times the average energy normally deposited by the incident electrons), they severely distort the proportional relationship between the energy deposited in the detector and the





number of detected incident electrons. This relationship is crucial to the interpretation of EM images. Therefore, in order to use the APS as an electron detector for cryo-EM, we will have to thin down the silicon substrate. Simulations show the extra energy deposited by backscattering events decrease to less than 1% for incident electrons of 300 keV if the silicon substrate can be thinned down to 30 μm or less. We are currently investigating different thinning techniques.

In the meantime, one would like to know the characteristics of such a thinned detector. Since in our experiment, we detect electrons one at a time, we can roughly reproduce the results from the thinned detector by selecting only events with small energy deposition (for example, less than 10 keV). The table at left shows a typical reading for such an incident electron at 300 keV. In these clusters, the significant pixel values are always grouped inside a 3 x 3 array centered on the pixel with the maximum value. In this and the table below, original data were obtained with an APS chip with a standard silicon substrate thickness (300 μm). Data were adjusted to account for the thinning of the substrate to about 30 μm by excluding events where the energy deposited was greater than 10 keV. In order to get the average reading distribution, we selected for each case a 7 x 7 array centered on the pixel with maximum reading. The pixel value at each pixel position was added to the sum of all values of the pixel in equivalent positions in previous cases. At the end of a run, this sum was divided by the number of cases i.e. the number of detected electrons. The table at right shows the average distribution of 1641 events found in 29967 frames where the energy deposited by 300 keV incident electrons was less than 10 keV. The average distribution has significant values only inside a 3 x 3 array centered on the maximum. By summing over this 3 x 3 array, we get the average read out value of 43 ADC units. Since the average noise is about $\sqrt{9}$ x 1.5 = 4.5 ADC units, one can see that the average signal-to-noise ratio of each detected electron is approximately 10:1.

X_1	4	0	0	4	-2	3	1
X_2	0	0	1	1	-1	0	-2
X_3	-2	0	0	7	1	1	1
X_4	0	-3	4	24	2	-1	0
X_5	-1	1	-1	7	2	2	1
X_6	-2	0	1	0	-2	3	-2
X_7	-1	-3	2	-2	3	1	-3

X_1	0	0	0	0	0	0	0
X_2	0	0	0	0	0	0	0
X_3	0	0	0	3	0	0	0
X_4	0	0	3	31	3	0	0
X_5	0	0	0	3	0	0	0
X_6	0	0	0	0	0	0	0
X_7	0	0	0	0	0	0	0

This detector also has a good spatial resolution. The projection of the average distribution shown in the tables on either the X or Y coordinate could be fitted to a Gaussian curve with a FWHM of 21 μm. This FWHM is due mostly to the fact that the incident electrons are distributed all over the central pixel. If we suppose this distribution to be Gaussian with a FWHM of 20 μm (the size of a pixel) then we can try to de-convolute the result and obtain a spatial resolution of about 7 μm ($\approx\sqrt{(21)2 - (20)2}$).

Using this same method, our data yielded a signal-to-noise ratio of about 10:1 and a spatial resolution of about 11 μm for both 200 and 400 keV beams.

The above results show that it is possible to use an APS to build a detector for cryo-EM with incident electron energy in the range of 200-400 keV, having a signal to noise ratio of about 10:1 and with a spatial resolution of about 10 μm FWHM. Since the APS circuit is comparatively straightforward, using a 0.25 CMOS process one can reduce the pixel size to 5 x 5 μm and produce a 4000 x 4000 pixel detector. By thinning the substrate down to 30 μm or less, one can eliminate almost all the backscattering events. Such a detector, once working, will make a large impact in the field of electron microscopy; specifically in cryo-EM, since in addition to its high signal-to-noise ratio and small spatial resolution, it also has high radiation tolerance.[10] Moreover, the APS can be made to have a very short read out time thereby providing data collection at a much higher rate than with a standard CCD based camera.

Acknowledgments I must thank the many people who have helped me during my career. For the work on the screenless precession camera, I want to thank Joe Kraut who suggested the problem and encouraged me. For the work on the multiwire area detector, I am indebted to Wayne Vernon, Ron Hamlin, Chris Nielson and Andy Howard. For the work on the silicon pixel array detector, I want to thank P. Datte and specially J. Millaud at LBNL. The coauthors of the work done with the APS are: Anna-Clare Milazzo, Philippe Leblanc, Fred Duttweiler, James C. Bouwer, Steve Peltier, Mark Ellisman and Liang Jin; from the UC San Diego; Howard Wieman, Howard Matis, Fred Bieser and Peter Denes from LBNL, and Stuart Kleinfelder from UC, Irvine. Last, but not least, I must thank my wife and daughter who have supported me for many years.

Nguyen-Huu Xuong

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The 9th Annual Structural Biology Symposium, UTMB Galveston, TX

The 9th Sealey Center for Structural Biology (SCSB) symposium: ***Proteins and Beyond: the Quest for Scientific Integration,*** was held at the University of Texas Medical Branch in Galveston April 30 - May 1, 2004. More than 300 scientists attended, including a group from the British Isles.

Combining information streams: systems biology: This first session began with a keynote speech from **Leroy Hood,** Head of the Institute for Systems Biology (Seattle). This institute has brought together scientists from many different backgrounds with the latest tools available to "decipher life." Combining genomics, proteomics, and structural biology allows one to take a global approach to determining pathway organization and the functional analysis of proteins in networks. One great advance is Isotope Coded Affinity Tags (ICAT) combined with mass spectroscopy. Leroy showed how this integrated approach could be applied to defining the approximately 100 mRNAs that differ between normal mice and those with cancer, and to analyzing the effect of *cis* regulatory elements in controlling gene expression. He also discussed the future of the "nanolab," where processes could be followed in a single cell.

Erin O'Shea (HHMI, UCSF) took up this point, while discussing the effects of stochasticity on interpreting results of assays in eukaryotic cells. Noise, or random disturbances in data collection can lead to irregularities in measuring expression levels of proteins in individual cells with fluorescence microscopy. The noise problem becomes more acute at lower expression levels. By measuring expression of two alleles, with two reporter genes in diploid cells, her group could show that noise is gene-specific and not dependent on the regulatory pathway or absolute rate of expression.

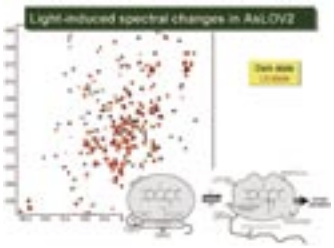
Adam Arkin (UC Berkeley) then discussed how non-linear and stochastic processes govern cellular response to stress. He showed some of the complex control mechanisms involved in cell survival, in the conservation of of enzymes needed for chemotaxis, or sporulation in bacilli. His group is applying concepts classically used by engineers and applied mathematicians, such as optimization or control theory, non-linear dynamics and stochastic process theory, to survey the data and make logical connections. This allows them to integrate a large amount of biochemical data into coherent pictures of the pathways. This integrative analysis should illuminate the fine tuned mechanism of adaptation that is required for a cell during its life cycle.

James Ferrell (Dept. of Mol. Pharm., Stanford) continued with control of eukaryotic cell cycle by patterns in protein activation and destruction. Theoretical and experimental studies can be used to understand the loops in signaling cascades. Extracts of Xenopus oocytes entering and exiting mitosis show a "positive feedback loop" of the cyclin B protein that triggers cell division. The regulator Cdc2 mediates activation of Cdc25 and inactivation of Wee1 and Mty1, causing the loop to have two stable points. Such oscillators with a bistable trigger (relaxation oscillators) would ensure that the mitotic oscillator would never approach intermediate steady state of "partial mitosis." More cyclin is needed to induce entry into mitosis than to maintain mitosis. Hysteresis in this bistable system would prevent the system from slipping back from mitosis to interphase. The significance of these studies lies in the fact that the complex regulatory mechanisms such as cell cycle are based on basic systems-level logic.

21st Century Structural Biology: Visualizing intracellular and multicellular interactions: Speakers in this session showed how advanced structural biology techniques can be used to visualize cell processes. For example, ***Wolfgang Baumeister*** (Max Planck Inst, Germany) uses electron tomography to visualize superamolecular architecture within cells. This is one of the few techniques available that yield medium range (nanometer) resolution of complexes within (unstained) cells. Recent advances in maximizing the precision and accuracy of the tilting device on which the sample is placed allow researchers to take a larger number of serial projections with less error. Denoising and averaging techniques could be used to minimize the cumulative electron dose across the sample during data collection, yielding detailed pictures at (4-8 nm resolution) of cellular machinery. The applications shown included virion particles within or outside cells, sea urchin sperm flagella, extension and retraction of filapodia by Dictyostelium (slime mold) grown directly on the EM- grid. The next plans are to use high-resolution structures, from methods such as crystallography or NMR, of cellular components to build supertemplates for cross-correlation searches in the tomograms, combined with fluorescence labeling.

Larry V. McIntire (Emory and Georgia Tech) illustrated how pressure and other external forces affect cellular interactions and gene expression. Understanding local mechanical forces can aid in the study of thrombosis and atherosclerosis, which occur in areas of the body with low flow shear stress and high cyclic strain. Monolayers of human umbilical vein endothelial cells and primary human aortic endothelial cells were placed in a parallel plate flow chamber with differing flow-shear stress (25 dyn/cm^2) and cyclic strain was applied to model the mechanical forces experienced by vessel walls. DNA microarrays indicated the genetic responses to these mechanical forces. Among these were several genes (but not nitric oxide synthase) in the NO production pathway. These gene products could supply new substrates for NO synthase (arginosuccinate synthetase) or be overall regulators of NO synthase activity (caveolin 1 and α-Galactosidase A). Genes important for maintaining an anti-coagulant state such as tPA, thrombomodulin, prostaglandin receptor 2, Cyp450 1A1 and 1B1 and COX2 were up regulated, while increased flow decreased the expression of PAI-1 and PAR-1. Some genes were up-regulated by shear stress but down-regulated by cyclic strain (endothelin,PAR-1 and MCP-1). These results provided new insights about the effect of cell-mechanical environment on genetic pathways.

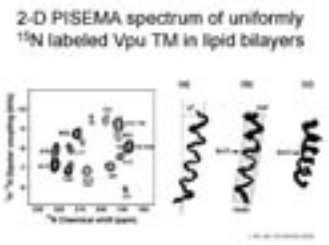
Dynamic proteins and their partners: In a return to the topic of how protein contacts control switch mechanisms in cells, ***Kevin Gardner*** (UTSW Medical Center, Dallas) showed how phototropins perform as "light switches." They combined



3D isotope-edited NOESY spectra, 15N/1H and 13C/1H heteronuclear single-quantum coherence (HSQC) spectra and 2H exchange protection to contrast the dark and light states of a PAS domain. Photo activation causes structural changes that propagate across to the conserved J α helix, while no gross structural deformations occur in the PAS core. Removing the last C-terminal 24 residues, a critical portion of J α helix, caused significant chemical-shift differences for residues located in the core. Together, these data provide a model for steps in the light-dependent signaling process used to specifically stimulate phototropin kinase activity upon exposure to blue light.

Robert Callender (Albert Einstein College of Medicine) showed further how protein dynamics contribute to catalysis, using relaxation spectroscopy of protein binding in the nano - to millisecond range. Transient perturbations of an equilibrated system can cause alterations in the IR absorption or UV/visible fluorescence that can be followed as the system returns to equilibrium. Such "laser-induced temperature-jump relaxation spectroscopy" was used to calculate kinetic constants for the active site loop motion of lactate dehydrogenase and triosephosphate isomerase; substrate binding constants so determined agreed well with NMR data. After the loop opens the ligand dissociation step is rate limiting, independent of temperature.

Mauricio Montal (UCSD) is using the Vpu protein from HIV-1 as a model for new methods to study transmembrane (TM) helical domains with NMR. They determined the structure and orientation of the TM-helices relative to the bilayer by a combination of solid-state and solution NMR methodologies such as the 2-D PISEMA (Polarization Inversion Spin Exchange at the Magic Angle) spectroscopy. They used TASPs (Template Assembled Synthetic Proteins) chemical synthesis methodology to link five Vpu TM domain monomers and showed that the ensemble had similar channel forming activity to the native Vpu protein. This work illuminates the role and molecular mechanism of Vpu in facilitating budding of new virions and could be the basis for design of anti-HIV drugs that block the Vpu channel activity.

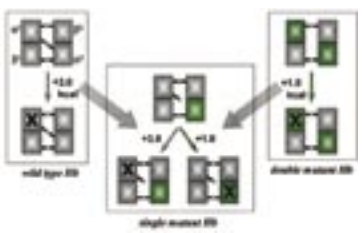


Bryan Sutton (UTMB) provided a lively interlude in the meeting, with a movie on how arrestin interacts with the photoreceptor rhodopsin, the prototypical GPCR, to stimulate transducin-mediated signaling. Phosphorylation of the C-terminus of rhodopsin allows arrestin binding, accompanied by the movement outward and up into the membrane of the amphipathic C-terminal α-helix of arrestin. There are many arrestins with differing receptor specificity. A single β-strand switch alters the specificity of the structurally similar β-arrestin, which binds non-visual GPCRs, and rod arrestin, which binds rhodopsin in rod cells. Understanding these evolutionary relationships may provide important information on the evolution of this and other families of regulatory proteins.

Lucas Tamm (U. Virginia) described how NMR can be used to study the folding and dynamics of *E.coli* outer membrane protein A (OmpA). While there are few structures of membrane proteins, they constitute 60% of all pharmaceuticals target proteins. Omp A has an 8- stranded β-barrel membrane domain, and a C-terminal periplasmic domain of unknown structure. The equilibrium folding of OmpA in this liposomes was monitored by fluorescence and by gel-shift assays, which showed that it is a two-state, reversible process. NMR studies in DPC micelles indicate that the transmembrane β-strands are well-defined, while the extra-membrane loops seem to be either intrinsically disordered or highly dynamic. Many of the residues that show significant backbone dynamics on the μs-ms time scale point inwards into the lumen of the β-barrel, Some of these residues form salt bridges and hydrogen bonds that obstruct the ion channel in the closed state but dissociate in the open state. Therefore, studies of the dynamics of membrane proteins by NMR could help elucidate the mechanism of ion channel function.

Ron Kaback (HHMI, UCLA) continued with the study of membrane proteins, revealing his "passion for permeases." He provided an insight into function using a 3.5Å crystal structure of lactose permease, a membrane protein in *E. coli*. Crystallization took several years due to the inherent flexibility of the molecule. The enzyme's flexible structure is probably needed for the permease to function in its native environment. While crystallization was only possible for a mutant that was locked into one conformation, plotting the position of hundreds of other known mutations on this structure revealed the differing conformations of the protein. His work again showed how integration of structural biology with biochemistry can reveal detailed information about how the regions of the protein function in its overall activity.

The symposium concluded with another talk on a protein that has been studied for many decades. **Gary Ackers** (Washington U, St. Louis) showed new details of the interactions within the hemoglobin (Hb) tetramer during oxygenation. There are 10 different partial to full oxygenated states of Hb, but detailed structures of the partial states have not been obtained. Previous models, which used data from symmetric mutants of hemoglobin, indicated that changes in contacts at the dimer-dimer interface mediated cooperativity. However, new data with "asymmetric" mutants, hybrid tetramers composed of one wild-type and one mutant dimer, indicated the oxygen affinity of the wild-type dimer was not altered, and thus that the structural basis of cooperativity must be within each dimer. Further work also indicates that the Bohr effect is mainly associated with intra-dimer communication. The conformational switch in



quaternary structure between the so-called tensed and relaxed state occurs as soon as both dimers have at least one oxygen bound.

Poster prizes: Posters were limited to 100 this time because of space constraints. The overall quality was excellent, as usual, and the judges again decided to award several first prizes in the graduate and postgraduate categories. The 200$ prizes were funded by the SCSB. The graduate student awards went to **Amy Williams** (U. Houston), **Zhen Zhang** (Baylor College of Medicine) and **Lavanya Rajagopalan** (UTMB). **Paul Blackburn**, from the U. Glasgow, Scotland, and **Josephine Ferreon**, **Scott Larson** and **Numan Oezguen** from the UTMB received the postgraduate awards.

Graham Randall, Baylor; Hongjun Jin, Texas A&M; Tara Davis, UT-Southwestern; Rodrigo Maillar, Andy Chen, Lavanya Ragopalan, Kerry Fuson, Payal R. Sheth, Jurg Roesgen, Josephine Ferreon, and Catherine H. Schein, UTMB

The next SCSB Symposium will be May 20-21, 2005, details can be obtained at: www.scsb.utmb.edu/

The 2005 ACA Summer Course in Small Molecule Crystallography.

This course will be offered June 5th - 15th, 2005 at the Indiana University of Pennsylvania, in the town of Indiana located about 80 miles east of Pittsburgh. There will be three lectures each morning on single crystal and powder diffraction methods, followed by afternoon and evening workshops for problem solving and for crystal structure determination. Attendees are encouraged to bring their own single crystal or powder samples for x-ray data collection. Attendees are expected to have at least an undergraduate science degree. 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).

Three Bruker-Nonius single crystal diffractometers (two CAD4's at IUP and an APEX instrument with CCD detector located at U. Pittsburgh which will be electronically linked to the x-ray Lab at IUP) will be available along with a Bruker-Nonius D8 powder diffractometer in the x-ray Lab at IUP and a Miniflex powder diffractometer on loan from Rigaku. There will be adequate computing facilities including access to the CSD and ICDD databases.

The organizers of this ACA Course will 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.

The organizers aim to have about 25 attendees; in past years they have come from academia (students and faculty), government and corporate institutions, and from the U.S. and other countries. We encourage applications from Latin America. Tuition will be $250 ($750 for those from Corporate Labs). IUP housing (includes breakfast and lunch) can be arranged for the duration of the 10 day course for an additional $400.

Up to twelve graduate student scholarships will be offered. These will consist of a waiver of tuition and campus housing costs with two meals a day. 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 aim to provide at least two scholarships specifically for Latin American graduate students. Scholarship awards will be announced by April 15th, 2005.

The Course registration form can be obtained from the ACA website: **www.hwi.buffalo.edu/ACA/**. Completed forms must be received before April 1st, 2005 by Bryan Craven, Chemistry Department, Indiana U.of Penna., Indiana, PA 15705, USA (or sent electronically to Charles H. Lake at **lake@iup.edu**). Student applicants must enclose a personal statement addressing the above three criteria. Also, the student's mentor is asked to mail separately to Professor Craven a letter of recommendation written on institutional letterhead. A check made out to "ACA Summer Course" for the total amount of tuition and housing (which must be drawn on a U.S. bank) must be received by Bryan Craven or Charles Lake by May 29th, 2005. Further information can be obtained from **craven@icubed.com** or **lake@iup.edu**.

The faculty and their research interests are:

Nattamai Bhuvanesh, Texas A & M. Solid state chemistry, powder diffraction.
Robert Blessing, HWI & SUNY, Buffalo. Structural Biology, Shake n Bake.
Bryan Craven, Indiana U. of Penna. (Co-organizer). Crystallography, charge density, neutron diffraction.
David Duchamp, formerly Pharmacia, Kalamazoo. Structures of small biomolecules, crystallographic software.
Steven Geib, U. Pittsburgh. Service crystallography of small molecules.
Curt Haltiwanger, Bruker Axs Inc., Madison, WI. Single crystal diffractometry and structure determination.
James Kaduk, BP Corp., Naperville, IL. Crystal structure determination from powder diffraction.
Jeanette Krause, U. Cincinnati,. Service crystallography of small molecules.
Charles Lake, Indiana U. of Penna. (Co-organizer). Inorganic structures, crystallographic teaching.
Thomas McNulty, RigakuMSC Inc., TX. Powder diffractometry.
Hamilton Napolitano, Universidade Estadual de Goias, Brazil. Structures of small bioorganic molecules.
Marilyn Olmstead, U. California at Davis. Crystallography of small molecules, crystallographic teaching.
Robert Stewart, Carnegie-Mellon U., Pittsburgh. Theory of x-ray scattering from crystals, charge density studies.
Brian Wargo, Freedom High School, Pittsburgh & graduate student U. Pittsburgh. Powder diffraction tutor.
John Woolcock, Indiana U. of Penna. Inorganic structures from crystallography and NMR.

Crystallography Web Watch

This column is a bit different from usual because none of the sites noted are crystallographic in nature. Rather it is concerned with environmental chemistry, especially green chemistry.

The Environmental Protection Agency has a web site that provides a great deal of information about a wide range of topics. One of their websites **www.epa.gov/nheerl/dsstox/** is entitled Distributed Structure-Searchable Toxicity Public Database Network. This new website contains chemical structure and toxicity information that can be searched though the data must be imported into a chemical relational database application in order to carry out the searching and analysis. Another of the EPA's web sites **www.epa.gov/eims/** offers access to a public archive of their published scientific reports and other documents. On this site, search tools are provided.

A third website **www.epa.gov/greenchemistry** gives entrée to the increasingly important area of green chemistry. This site gives a nice sense of the breadth and defining principles of green chemistry, as well as tools and funding opportunities. The Green Chemistry Institute at the American Chemical Society **www.chemistry.org/portal/a/c/s/1/acsdisplay.html?DOC=greenchemistryinstitute\index.html** maintains a web site that gives information about meetings, research funding opportunities and information on schools that have programs in green chemistry. A who's who of scientists influential in this area is maintained at **www.uoregon.edu/~hutchlab/greenchem/beyondoregon.html**, and **www.nsfstc.unc.edu/green.htm** gives links to many green chemistry organizations.

The field is growing in significance. The Royal Society of Chemistry has published a journal, ***Green Chemistry since 1999;*** see **www.rsc.org/is/journals/current/green/greenpub.htm**. Abstracts of review articles can be found on-line though articles must be purchased. There have been Gordon conferences on green chemistry since at least 1999. The list of speakers and topics for the summer 2004 conference **bama.ua.edu/~rdrogers/GreenChemistryGRC04/** gives a sense of the breadth of the field.

There are growing numbers of colleges and universities offering courses and degrees in green chemistry. The University of Scranton, for instance, has put together a useful web site **academic.scranton.edu/faculty/CANNM1/greenchemistry.html** that includes a number of links that would be helpful to someone teaching undergraduate chemistry. The site also includes teaching modules that allow the insertion of green chemistry into a number of standard chemistry courses. Some students might want to pursue a co-op or internship in green chemistry and this site should be helpful to them – **www.chemstudent.com/green_coop_all.htm**.

If you have a favorite web site that you'd like to see in a future **Crystallography Web Watch** column, please send the web address and a brief description to **Kay Onan (k.onan@nunet.neu.edu).**

Bruker AXS Party at the Museum of Science and Industry, Chicago ACA 2004

Ccwise from top right: Bill Ojala with Engine; Jeff Deschamps and Herb Hauptman; around table from left: Gregory Ferrence, Bob McDonald, Gary Enright, Michael Jennings, and Jim Britten; Michael Carducci, Sue Byram and Patrick Bryant; Qi Gao, Laura Kelley and Nancy Tsou; Fred Hollander with fantastic looking vehicles. All photos were contributed by Victor Young.

Mentor-Mentee Dinner at Chicago ACA 2004

Thanks to the partial support of Hampton Research, Nextal and Fluidigm, this popular event was held at the Blue Agave Restaurant. Middle, from left: Robert Heuther in intense discussion with I.David Brown; Chris Fleming, Sompop Bencharit and Judy Flippen-Anderson seated in booth; Bottom row from left: Tom Furnas with Anna Gardberg; Charlie Weeks and Joel Bernstein.

Above: Tina Izard and Charlie Carter.

At right: Jeff Wilson, Matt Vetting, Deb Breiter and Jeff Habel.

MSC / Rigaku Fun Run at Chicago ACA 2004

All athletically inclined crystallographers should be pleased to hear that another MSC / Rigaku - sponsored Fun Run will be held at the ACA Meeting in Orlando.

The group photo at top was contributed by Sue Duncan; the others were taken by Judith Flippen-Anderson.

Alberto Podjarny at the Mar USA Party at the Blue Chicago Nightclub (ACA 2004). Photos courtesy of Ross Doyle.

In view of these and the preceding pages full of people having fun at the ACA 2004 meeting - how can anyone resist coming to ACA 2005 in Orlando??

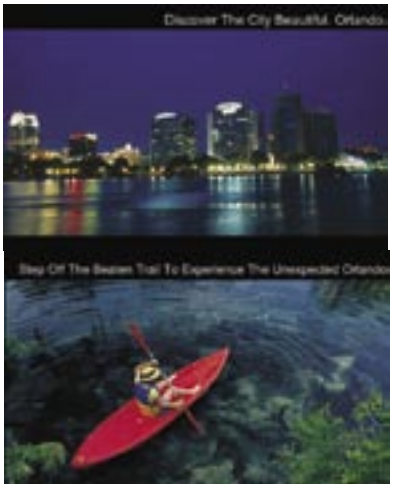
ACA 2005 May 28 - June 2 Walt Disney World Swan Hotel

www.xray.chem.ufl.edu/aca2005/index.htm

2005 Program Chair:

Ed Collins

edward_collins@med.unc.edu
919-966-6869
fax 919-962-8103



2005 Local Chairs

Khalil Abboud (at left)

abboud@chem.ufl.edu
352-392-5948; fax 352-846-2040

Tom Selby

tselby@mail.ucf.edu
office: 407-823-6752; lab: 407-823-1115

Photos courtesy of Orlando/ Orange County Convention & Visitors Bureau.

Meeting Calendar

MAY 2005

19-29 **Evolving Methods in Macromolecular Crystallography,** 37th crystallography course, Erice, Italy. **www.crystalerice.org/futuremeet.htm**

24-28 2nd International Conference on Photo-Induced Transition, U. of Rennes1, France. Contact: **gmcm-pipt@listes.univ-rennes1.fr; www.gmcm.univ-rennes1.fr/pipt/**

MAY / JUNE 2005

28-2 **ACA Annual Meeting, ACA 2005, Walt Disney World Swan Hotel, Orlando, FL. www.xray.chem.ufl.edu/aca2005/index.htm Local Chairs: Khalil Abboud, abboud@chem.ufl.edu, and Tom Selby, tselby@mail.ucf.edu; Program Chair: Ed Collins, edward_collins@med.unc.edu.**

AUGUST 2005

18-23 **IUCr Computing School** (prior to IUCr Congress), in Siena, Italy.

23-31 **XX IUCr Congress**, Florence, Italy. **Local Chair:** Paola Paoli, **iucr@iucr2005.it**, **Program Chair,** Carlo Meali, **www.iucr2005.it**

OCTOBER 2005

6-7 **International Workshop: Watching the Action: Powder Diffraction at non-ambient conditions.** Max-Planck-Institute for Solid State Research, Stuttgart, Germany. Contact: R.E.Dinnebier, B.Hinrichsen & M.Jansen, **www.fkf.mpg.de/xray/**

NOVEMBER 2005

6 –10 **Sociedad Venezolana de Cristalografía** (SVCr) is planning a full day session at the next congress of **Sociedad Venezolana de Química** (SVQ), Mérida, Venezuela. An advanced course on Powder Diffraction will be conducted as a satellite activity of the Congress. For more information, please contact: Graciela Díaz de Delgado: **diaz@ula.ve** (SVQ-SVCr meeting) or Miguel Delgado: **migueld@ula.ve** (PD course).

JUNE 2006

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

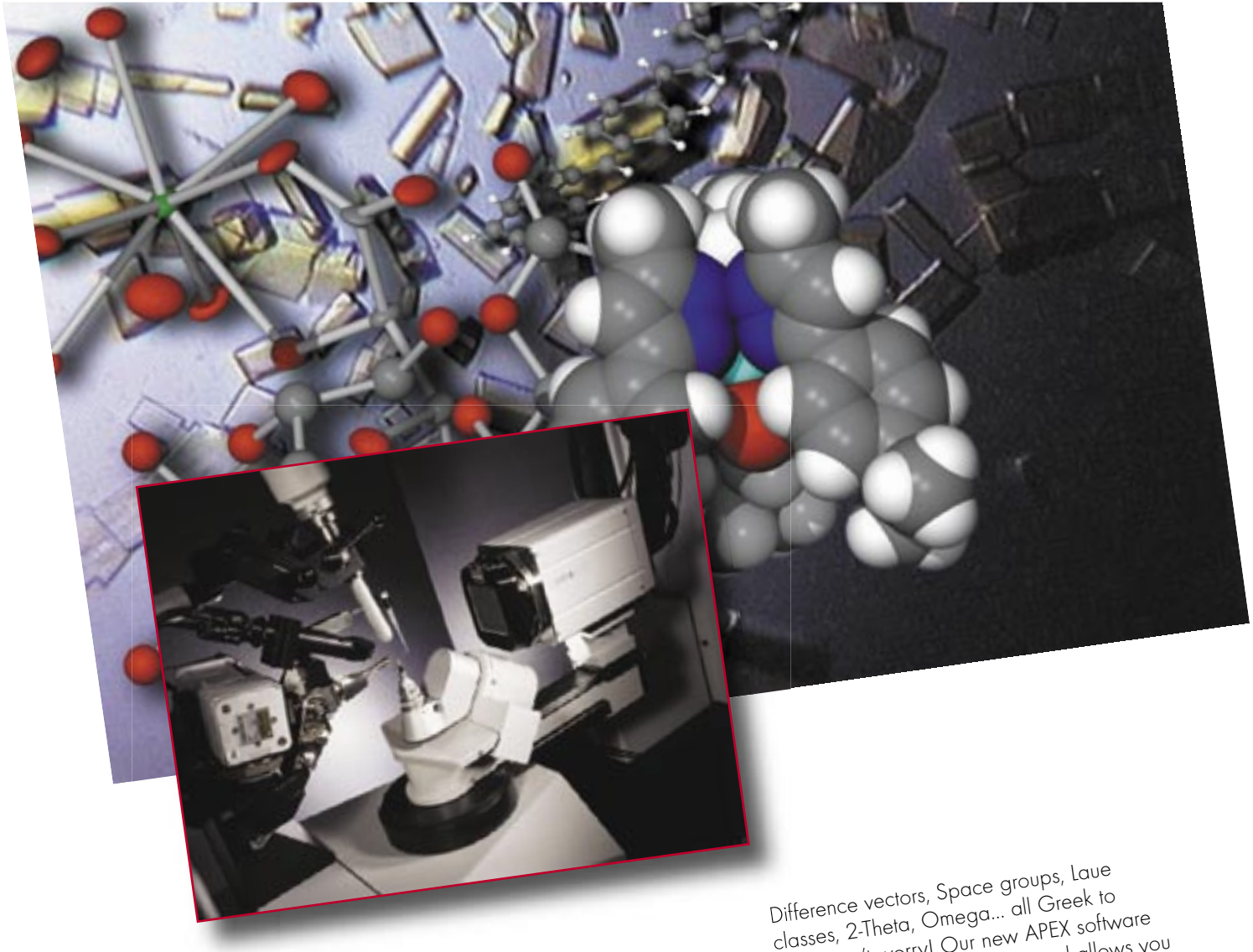
JULY 2006

22-27 **ACA Annual Meeting, ACA 2006, Sheraton Wakiki, Honolulu, Hawaii.**

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.

Please Note: A postdoctoral position in the area of crystal growth in the Condensed Matter Sciences Division at Oak Ridge National Laboratory has recently become available. Experience in the Czochralski growth of single crystals is particularly desirable. Postdoctoral appointments at ORNL are generally from one to three years in duration as determined on an annual basis. U.S. citizenship is required for this position. Interested parties should contact Lynn Boatner at **boatnerla@ornl.gov** or tel. 865-574-5492.



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Generator	Optic	Normalized Useable flux*	d_{max} (Å)†
RU-H3R	Blue	1.00	270
MicroMax™-007	VariMax HR	2.94	314 - 430+
MicroMax-007	VariMax HF	3.92	246 - 400+
FR-E SuperBright	VariMax HR	7.34	314 - 525+
FR-E SuperBright	VariMax HF	9.81	246 - 500+

* Normalized, calculated flux through a 0.3 mm pinhole at the crystal position
† Calculated longest resolvable unit cell on an R-AXIS IV++ at 300 mm XTD

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VariMax: Patent pending

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