American Crystallographic Association

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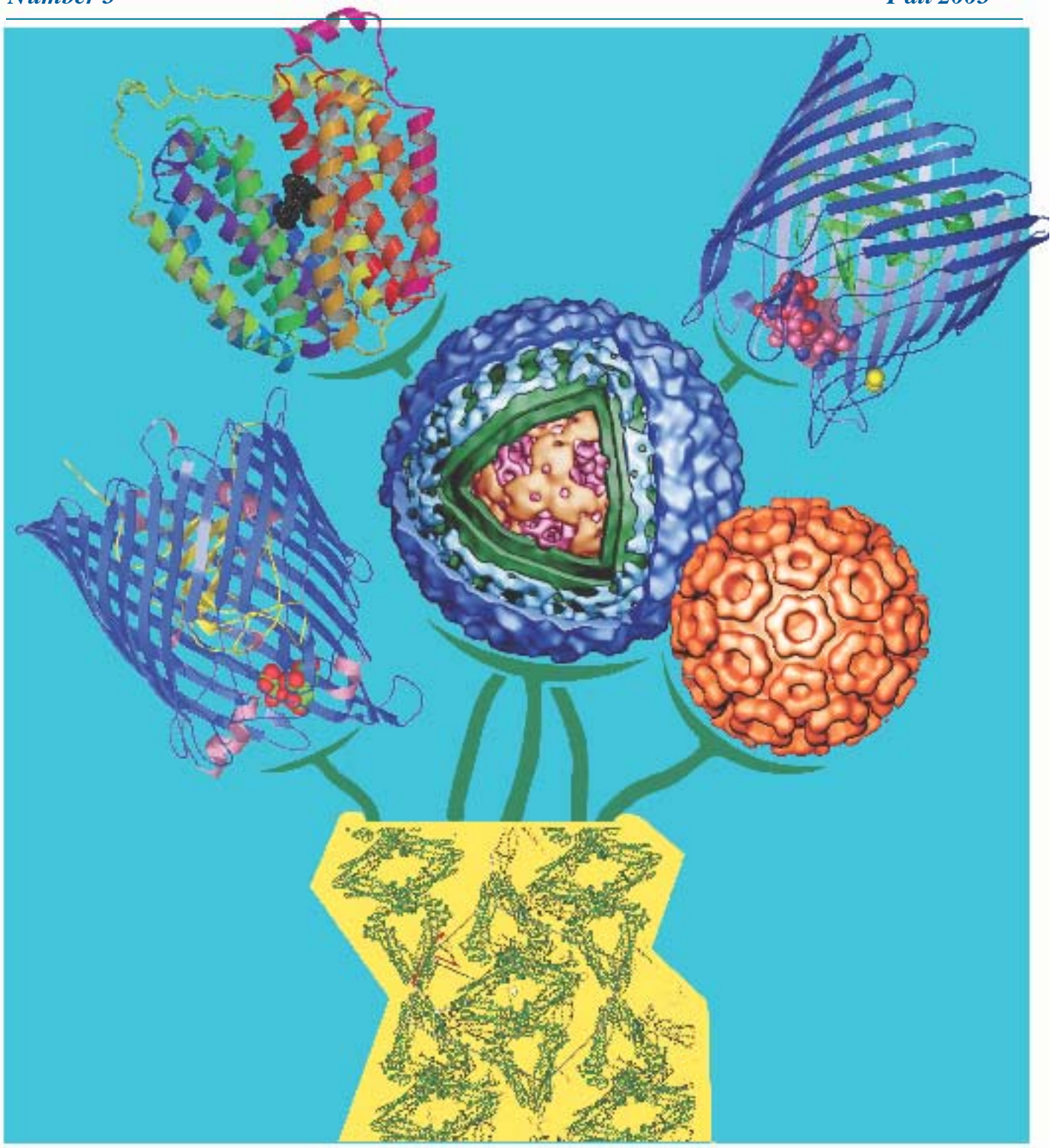

Membrane Protein Structures

Northern Kentucky ACA Meeting

Table of Contents

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President's Column

I write this column with happy memories of our quite successful annual meeting just concluded in Covington, Kentucky. Much of this *Newsletter* is devoted to reports of that meeting, and I thank those who contributed those reports in such timely fashion. The meeting arrangements by the local committee, both logistical and social, were well thought-out and cleanly executed, and I can't imagine a meeting running more smoothly. I'm sure the more than 900 participants in the Covington meeting join me in thanking Bobby Barnett and his local committee for their hard work. The Northern Kentucky Convention Center provided a combination of comfortable ambience for a meeting the size of ours and ready responsiveness to inevitable last-minute changes. This experience suggests to ACA Council that such mid-sized convention facilities can be especially suitable for our meetings, and comparable venues are bound to receive close consideration for future meetings. The entire social program was varied and pleasant, from the opening reception at the Newport Aquarium, through the traditional awards banquet, to the Ohio River dinner cruise at the meeting's end. A special word of thanks is due to the social events local subcommittee headed by Ann Wolff for arranging these pleasant events. Science and the arts were combined in Charlie Carter's Past President's address at the banquet in a novel and artistic way that none present will soon forget. What an act to follow (but don't get your hopes up)!

The scientific program, consisting of more than 500 presentations, was exceptional, and its balance and scope as arranged by Jeanette Krause Bauer, her program committee, and the SIG chairs, set a high standard of efficient scheduling and execution. (My biggest program disappointment, not attributable to the program committee, was the distressingly large number of vacant poster slots and the too-frequent absence of poster presenters - even some otherwise eligible for Pauling or Oxford Prizes - at their scheduled discussion times.) An intensive five-hour session of planning in Covington by the 2004 local and program chairs, the SIG representatives, and the ACA Council has already laid a firm foundation for our Chicago meeting next year.

The presentation of major ACA awards to **Jim Ibers** (Buerger Award), **Takeshi Egami** (Warren Award), and **Julia Chan** (Etter Early Career Award) with their associated symposia represented another meeting highlight on both personal and scientific grounds. The *Transactions* Symposium on Biological Neutron Diffraction, the special symposia on Time-Resolved Diffraction and on Crystallographic Computing, and the workshops gave stimulating update and focus to innovative areas of crystallography, and I thank the organizers for their work in arranging these special sessions. (con't, page 5)

The names of recipients of three ACA awards to be presented in Chicago next year were announced in Covington. Congratulations to **Alexander McPherson** (the Isidor Fankuchen Award), **Dick Marsh** (the first Kenneth N. Trueblood Award), and **Nguyen-Huu Xuong** (the new Charles Supper Award). We can all look forward to symposia in Chicago developed around the research and interests of these three outstanding colleagues. *(See pages 9 and 11 for more details.)*

Recognition of students took many and varied forms at this meeting. In addition to the now-familiar Etter Student Travel Awards, the Pauling Poster Prizes and the Oxford Poster Prize, some new forms of student recognition were seen in Covington. These included the new Protein Data Bank Prize to a student poster presenter, and the designation (with accompanying cash awards) of several student speakers as Margaret C. Etter Student Lecturers. *(See pages 13-15.)*

The exhibition of the latest instrumentation and techniques was the best and largest ever, with more than 125 participants representing more than 40 exhibitors (an ACA meeting record). Corporate memberships, now 36, are also at an all-time high. The smooth execution of this perennially excellent exhibition is due in large part to AIP's Bob Finnegan, who manages our exhibition each year. Our exhibitors and corporate members contribute immeasurably to the success of every annual meeting, scientifically, financially, and socially. While their financial and social contributions are most evident during the meeting, the benefits of their contributions to our science last all year. I know you join me in thanking them for their continued support of ACA.

This year's meeting also saw a continued expansion of our interaction with crystallographers from Mexico and from Central and South America. The presence in Covington of Iris Torriani of Brazil, who is the regional representative from the IUCr, gave welcome opportunity for a fruitful exchange of views with members and with ACA Council. The Council continues to explore ways to strengthen these ties, including the suggestion that a provision for country memberships in ACA might provide an economical way to spread the benefits of ACA membership southward. Along these lines, you will be interested to read Charlie Carter's guest editorial about his recent scientific visit to Cuba.

We are saddened by the deaths of our colleagues Elizabeth Holt, Jim Holden, and Ron Burns, reported in memorial articles on pages 22-23 of this *Newsletter*.

Finally, I call your attention to the upcoming ACA elections. Candidates for ACA offices were presented in the Summer 2003 *Newsletter*. Ballots will be distributed to the membership in mid-October, with a deadline of November 15th for submission. There was discussion at the business meeting in Covington about eliminating the long-standing requirement that applicants for ACA membership must be recommended by two present ACA members. This involves a change in the ACA bylaws, and a motion to put this proposal to the required vote of the ACA membership was approved by a majority of members present at the Covington business meeting. You will see that issue on your ballot when it arrives. I note that fewer than a quarter of our members have typically voted in the past few ACA elections. Though this fraction is higher than in many other elections, I hope for a higher turnout from ACA members this fall. Please give this election your thoughtful attention, and note that electronic balloting will be available.

Ray Davis

Guest Editorial: ACA Past-President Charlie Carter

"I believe there is a transcendent, international society of decent people," Carlos was saying, "and Augustin is a charter member of that society." My wife Valerie and I were driving with Carlos Rodriquez, and Ernesto Estévez to luncheon at El Palenque, a restaurant off Fifth Avenue in West Havana serving quintessential Cuban food and whose name describes the outposts of runaway slaves during the prolonged slave labor on sugar plantations. Carlos and Ernesto are, respectively, Director and Vice-Director of the Institute for Materials Sciences, an adjunct of the Physics Department of the University of Havana. Ernesto, our host and guide, is an animated storyteller with an encyclopedic command of history and science. He had invited me to participate in their IUCr summer school in Materials Science, which ran from 6 to 24th July. We visited Havana from 6-13 July with the support of the IUCr as part of the Latin American Initiative.

This letter distills my experiences and impressions from that week. I hope to correct some of the distortions of Cuban society advanced by the US government and media, and to encourage others to visit and learn about Cuban science. Who better than the crystallographic community to promote cooperation among scientists internationally.

Carlos was describing his best childhood friend, Augustin Lage, who I would meet the next day. Augustin had become an immunologist when Carlos chose physics, and the two often joked about who had made the correct choice. "Augustin is the smartest human being I know," Carlos continued, "and he is especially wonderful because he never lets his intelligence get in the way of having each conversation reach its fullest potential." *(con't, next page)*

As I found nearly all Cuban scientists to be, Carlos, Ernesto, and Augustin are upbeat realists whose imagination, subtlety, and humor belied any suggestion that they felt "repressed." We were in the midst of a phenomenon that Valerie was to identify with precision for me when we returned home: "their inner life is exactly like ours," she said. Indeed, Carlos and I knew almost without speaking what was in the other's thoughts. As was true also for Ernesto, Carlos would not let the hardships he dealt with on a daily basis interfere with our communication. It was the beginning of a lovely afternoon.

Over our lunch of roasted pork, Cuban rice and beans, and Bucanero beer, Carlos introduced me to the Cuban biotechnology industry, which was launched early in the game because of an outbreak on the island of Dengue fever. This was combated effectively by the development of a vaccine, which subsequently lead molecular immunology to flourish in Cuba. Several other important vaccines, including a promising and unique synthetic vaccine against *H. influenzae* and a rather effective new "vaccine" against some forms of cancer soon followed. The latter is so promising that, somewhat hypocritically, the US government has made an exception to the embargo to enable its use by US patients.

The next day, I learned from Ernesto Moreno at the Center for Molecular Immunology that biotechnology products sold to Europe and the third world bring in $100 million annually, and that this figure should rise sharply as some of the innovative products now in advanced clinical trials come to the market. Much of this income is re-invested in the industrial parks of West Havana, which already are the pride of the Cuban research community. Macromolecular crystallography is urgently needed here. Guy Dodson ran a successful protein crystallography workshop here several years ago, and the Moreno group has produced their first crystals of an antibody:hapten complex related to a potential product. The student who had grown them has a very sophisticated understanding of the physical chemistry of crystal growth, as well as a healthy skepticism about the quality of these crystals, which looked lovely to me. Cuba has a burgeoning collaboration with protein crystallographers in Göthenberg, Sweden, but because Cuba does not possess even a rudimentary photographic apparatus for characterizing the diffraction from such crystals, they often transport unsuitable crystals to Sweden, risking disappointment.

There seems to be an imminent collaborative liaison between immunologist and physicist/crystallographer. The two Ernestos (Moreno and Estévez) are approaching critical mass. I may have helped catalyze their emerging collaboration when I told Ernesto Estévez that proteins were studied as rigorously by single crystal studies as were small molecules. That made it more attractive to him to try macromolecular crystallography!

I actually met a third Ernesto, of the same generation, and was told that the frequency of Ernestos was a tribute to Ernesto Che Guevara, who is widely revered by all Cubans, perhaps second only to Jose Marti. All were proud to be his namesake. It seems relevant to point out at this point that the Cuban government is markedly different from others with which it is compared in the US media. Although flamboyant, Fidel Castro is hardly a narcissistic despot, and though his pronouncements are evident in many public places, he has a profound respect for Cuban history, of which he is an eloquent student. Moreover, domestic decisions are made by a meritocracy of gifted people in ways that are quite independent of Castro's continued presence. Two examples struck me. The first came in an article in *Smithsonian,* about Cuban natural resources: their "green" management policies. These policies have sustained the highest bio-diversity in the western hemisphere, and are essentially the creation of Alberto Perera, an eighty-one year old biologist. The second example involves the restoration of Old Havana. The old city is a treasure similar in many respects to Jerusalem in the opposite hemisphere. It is the oldest continuously occupied city in the new world, and as such has examples of each successive architectural style. The restoration is well advanced, and is contributing significantly to the growth of tourism. It is almost entirely the brainchild of Eusebio Leal Spengler, an outstanding architectural historian and artist, who single-handedly convinced UNESCO to invest in saving it from the advanced decay. Old Havana is a splendid place to walk, and the restored spaces include a spectacular camera obscura, which affords a 360° view of the city and harbor.

The talent and relative independence of these two administrators is consistent with the view, expressed by many, that little will change fundamentally in Cuba when Castro is gone. Cubans, by and large, are intensely proud of what they have accomplished in spite of US attempts to destroy their economy. Surprisingly, they seem to have neither time nor inclination to resent their megalithic neighbor to the north. It is difficult for the visitor to fault either the nobility of the Cuban social dream or the vitality of its implementation.

I found much to indicate that the caliber of Cuban science is of a high order indeed. Struggling under the US embargo, they nonetheless manage to grow projects through collaborations in Europe and elsewhere in Latin and South America, especially at the Campinas synchrotron. Another plea made repeatedly to me concerned online access to current literature. I mention this because the IUCr is in a position to provide such access to its journals by a number of different mechanisms. Those who sympathize with doing so should communicate their wishes to IUCr President Bill Duax.

There are important practical messages for US crystallographers. I had met Carlos Rodriguez the previous day, when he convened a group of scientists from physics, chemistry and biotechnology faculties, all of whom had an interest in x-ray crystallography. We discussed general problems and possible ways in which the American crystallographic community and in particular the ACA might form stronger relationships with Cuban scientists who have similar interests. All were particularly interested in increasing the participation of North American scientists in scientific meetings organized in Cuba. Luis Montero, chemistry professor and bioinformatician made the point succinctly when he said, "I feel insulted not to have contacts with an important scientific community!" Upbeat realism.

Coming up are four opportunities at which the attendance of American crystallographers could foster the growth of such relationships. These meetings, together with contact information in Cuba include: the Cuban Chemical Society Meeting, *(con't, p 9)*

Guest Editorial, con't

(Georgina Agüero, (a professor of inorganic chemistry), **yuyi@fq.uh.cu**); SLAFES (Simposio Latinamericano de Fisica del Estado Solido), a symposium in solid state physics, 6-9 December, 2004, with a possible satellite meeting, (Carlos Rodriguez, Director, IMRE, **dir@imre.oc.uh.cu**); a meeting early in February, 2004 devoted to "Molecular Design and Bioinformatics," (Luis Montero, Centro Virtual de Bioinformatica, **luis.Montero@fq.uh.cu**); and a school in protein crystallography which is in planning stages, (Ernesto Estévez, IMRE, **eerams@yahoo.com**). Any for whom these meetings would be appropriate are urged to contact either myself (**carter@med.unc.edu**) or the appropriate organizer.

It is entirely legal for US citizens to visit Cuba. A 1960s Supreme Court decision ruled it unconstitutional to legislate against travel by a citizen to anywhere in the world. Faced with this ruling, right-wing interests successfully passed a law preventing US citizens from spending any US currency in Cuba, and the administration of this law by the Treasury Department constitutes the only significant barrier to visiting Cuba. Nonetheless, my trip was entirely legal by virtue of three exceptions to this policy. First, there is a general license that may be used by any citizen bearing an invitation to visit Cuba for the purpose of participating in academic or intellectual programs. Second, specific licenses are granted by most academic organizations, which provide paperwork assuring that the costs of such visits do not constitute a violation of the Treasury policy. Finally, anyone can visit if their expenses are fully assumed by a host in Cuba. A slim volume: *Advice for Travelers to Cuba,* available from The Center for Constitutional Rights, 666 Broadway, New York, NY 10012; 212-614-6464; **ccr@igc.apc.org**, is highly recommended.

Every effort should be made to bring about more open and productive bridges between the US and Cuban communities. I hope that ACA members will make contacts with Cuban scientists and participate in their meetings. The exchange of knowledge by personal contacts is an obvious benefit, but in addition some progress might be made towards obtaining access for Cuban scientists to training in the US.

Charlie Carter

Letter to the ACA

Edith Hauptman and Ruth Clearfield at the ACA meeting opening reception.

Dear Marcia,

As per our recent conversation, I am writing to formally thank you and the committee for the excellent accommodations that were arranged in Cincinnati. In particular, I want to laud the ACA for the great job they do each year in negotiating the best possible room rates for the attendees. As an experienced conference attendee, I always check to see if I can negotiate a "better" rate and have not ever been able to do so. By contrast, the American Chemical Society does not pass on the best rates to its attendees, and I almost always am able to negotiate a better rate than the ones they offer. Kudos to the American Crystallographic Association for assuring the best interests of its members and not necessarily a kick-back for themselves. Abe & I are most appreciative.

Marcia, a special thanks to you for all you do to help make the meetings so enjoyable. the organization is truly blessed to have you in its employ.

Sincerely, Ruth Clearfield (Mrs. Abraham)

First Charles Supper Award to Nguyen-Huu Xuong

The ACA Council is pleased to announce a brand new award, the **Charles Supper Award**, to recognize scientists who have made exceptional contributions to crystallographic instrumentation. The Council is delighted to be able to announce simultaneously the the first recipient of this award, **Professor Nguyen-Huu Xuong**, University of California at San Diego, the well known pioneer of multiwire area detectors. This immediate link between award and first recipient is testimony to the high regard that the crystallograpy community has for Professor Xuong. See the upcoming winter *ACA Newsletter* for the full citation honoring him.

Charles Supper emigrated from Germany to the United States in 1925, bringing with him an ability to fabricate almost anything mechanical. While at M.I.T. during the late 1930s, he collaborated with Martin Buerger in the development of the precession camera. This instrument was to become the most significant single-crystal camera of the second half of the century. By 1941, he recognized the need for a company to manufacture and supply high quality, easy-to-use, reasonably-priced instruments for the x-ray crystallographer and he founded the Charles Supper Company. Mr. Supper's innovative designs and methods led to the commercial availability of the Buerger precession cameras, the Weissenberg camera, Debye-Scherrer powder cameras, goniometer heads, devices to fabricate crystal and protein models, film measuring instruments and other useful diffraction accessories. In the mid 1960s, the firm also became a major distributor for various crystallographic products created by others. The Supper award is given intermittently and consists of $1,000 honorarium to present a lecture at the Annual ACA Meeting. The Charles Supper fund was established by his son, Lee, in appreciation to the community of x-ray diffraction scientists for their continued support throughout the years.

2004 Fankuchen Award to Alexander McPherson

The **Isidor Fankuchen Memorial Award** recognizes the contributions to crystallographic research by a scientist who is known to be an effective teacher of crystallography. With great pleasure the award committee (Marilyn Olmstead, Hugo Steinfink, Abraham Clearfield and Joel Oliver) announces that the recipient of the 2004 Fankuchen Award is **Professor Alexander McPherson** of the University of California at Irvine.

Alex received his undergraduate education at Duke University and his doctorate from Purdue University under the direction of Michael Rossman. He did postdoctoral research at MIT in the laboratory of Alexander Rich, and then joined the faculty of Pennsylvania State University where he was promoted to Associate Professor. After Penn State Alex moved to the University of California at Riverside where he attained the rank of Professor and Chair of the Department of Biochemistry. In 1997 he joined the faculty of UC Irvine as Professor.

Throughout his career Alex has vigorously pursued protein crystallography, especially the theoretical and practical aspects of the crystallization of biological macromolecules. The biological systems investigated in his laboratory have included plant viruses, nucleic acids, immunoglobulins and numerous enzymes. The results of these investigations have been documented in over 275 publications that he has authored or co-authored.

Alex' contributions to education have also been exceptional. He has authored three books, one of which, *The Preparation and Analysis of Protein Crystals,* continues to be a major source of practical advice for growing protein crystals. He has been very active in organizing crystallization workshops and conferences for many years, having participated in more than 20 such events during the last ten years. For the past 15 years he has been an instructor at the Cold Spring Harbor Summer Course in Macromolecular Crystallography and thereby has helped train many young scientists. His former students have gone on to run major laboratories throughout the world and have trained many other leaders in the field of macromolecular crystallography. Most recently he has been an instructor in outreach programs to high school students, 1500 science teachers and the general public.

An outstanding teacher makes a deep impact in the lives of his protégés. Alex clearly qualifies for that distinction and the honor of the Fankuchen Award for 2004. *Joel Oliver*

The **Fankuchen Award** was established in 1971 in memory of Isidor Fankuchen, Professor of Physics at the Polytechnic Institute of Brooklyn from 1942 to 1964. It is given to recognize contributions to crystallographic research by one who is known to be an effective teacher of crystallography. Previous winners were: **2001: James Stewart; 1998: Eleanor Dodson; 1995: Jenny Glusker and Kennth Trueblood; 1992: Donald Casper; 1989: David Sayre; 1986: Michael Rossmann; 1983: Lyle Jensen; 1980: David Harker; 1977: Dorothy Hodgkin; 1974: Andre Guinier; 1971: Martin Buerger.**

First Trueblood Award to Richard E. Marsh in 2004

The first **Kenneth N. Trueblood Award,** which recognizes exceptional achievement in computational or chemical crystallography, will be given to **Richard E. Marsh,** Senior Research Associate in Chemistry, Caltech. Dick will give the keynote lecture in the Trueblood Symposium to be organized in his honor during the 2004 ACA Annual Meeting.

The Trueblood award was established in 2001 in memory of Professor Kenneth N. Trueblood, at the suggestion of many of Ken's colleagues, students and friends. Ken taught at UCLA 1949-1998, where he was recognized as an outstanding teacher and mentor. He was also a major force in the early use of computers and the development of crystallographic computer programs. Ken's early work on crystallographic programming is highlighted by possibly the first transatlantic collaboration with Dorothy Hodgkin and Jenny Glusker in the determination of the vitamin B12 structure.

There is no doubt whatsoever that the Trueblood Selection Committee: **Jenny Glusker,** Chair, **Bryan Craven, Katherine Kantardjieff and Bobby Barnett,** made a most appropriate selection when they decided to give the very first Trueblood Award to Dick Marsh. However, due to the siren call of summer vacations, and the short time between the selection and the *Newsletter* deadline, the formal citation that will more properly describe all the good reasons for choosing Dick will appear in the winter *ACA Newsletter.* Meanwhile, this is a good opportunity to include a less formal photograph of Dick Marsh - obviously at ease during his own annual summer vacation in Michigan.

Presentation of the Buerger and Warren Awards at the 2003 ACA Meeting Symposia

At left: Jim Ibers receiving the Martin J. Buerger Award from ACA President Ray Davis.

At right, Takeshi Egami receiving the Bertram J. Warren Award in Diffraction Physics before his lecture.

The Martin J. Buerger Award lecture: ***Less Difficult But Still Not Easy*** was given by **Professor James A. Ibers** at a Symposium in his honor organized by William A. Duax. Excerpts from his delightful lecture may appear in the spring 2004 *ACA Newsletter.*

The Warren Symposium, honoring **Professor Takeshi Egami,** was organized by Simon Billinge (*see report, page 32*). The winter 2003 *ACA Newsletter* may have exerpts from his fine lecture: ***Democracy in the Imperfect World: Local Crystallography of Crystals with Disorder.*** See the fall 2002 *Newsletter* for the citations and more details about these awards.

Margaret C. Etter Early Career Award Presented to Julia Chan

This award recognizes achievement and future potential among those at an early stage in their independent careers. It was established to honor the memory and celebrate the scientific accomplishments and mentoring skills of the late Margaret C. Etter, who was a Professor in the Chemistry Dept. at U. Minnesota. The award was given for the first time to **Julia Y. Chan**, PhD, Asst. Prof., Dept. of Chemistry, Lousiana State Univ., Baton Rouge, LA, in recognition of her outstanding achievements in the study of materials chemistry using crystallographic methods, her excellent leadership in teaching and mentoring, and her exceptional potential to continue to impact crystallographic research and education. Julia presented her award lecture: ***Structure-Property Relationships of Superconducting and Heavy Fermion Intermetallics*** at the Etter Award Symposium which was organized by Jeanette Krause Bauer and chaired by Carolyn Brock.

In addition several students were chosen by Special Interest Groups to receive the first **Etter Student Lecturer Awards**. They are (left to right in the photos): **David Lodowski** (Biological Macromolecules) ***Structural Basis for the Regulation of GPCR Signaling: the Crystal Structure of the GKR2:G-βγ Complex***; **Monica Allain** (Small Angle Scattering) ***Small-Angle X-Ray Scattering Measurements of Hydrogen Evolution from an Epitaxial Nb Film;*** **Peter Chupas** (Materials Science) ***Rapid Acquisition Pair Distribution Function Analysis (RA-PDF): Application to Time Resolved Structural Studies;*** **Jennifer Padilla** (General Interest) ***Generating Symmetry: Observed Macromolecular Crystal Contacts Explain Space Group Frequencies;*** and, receiving his award from Session Chair Xiang Ouyang, **Firas Awwadi** (Small Molecules) ***The Role of the Aryl C-Br ··· X- Synthon in the Crystal Structures of Copper(II) Halide Salts***.

Pauling Prize Committee Report

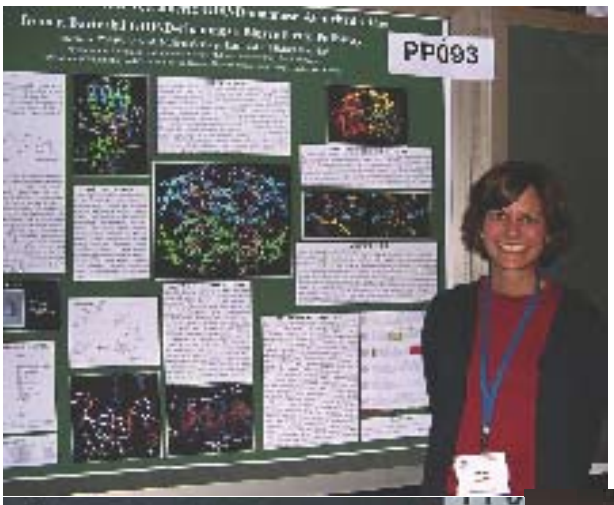
The Pauling Prizes, in honor of the late Linus Pauling, are given annually to graduate students who, by their poster presentations, demonstrate a high degree of knowledge, originality and perseverance in their research. Prizes include a copy of Pauling's *General Chemistry*, and a check for $200. No more than five prizes are awarded each year, and this year almost 60 posters were entered in the competition, making the job of judging difficult, but rewarding.

The general level of presentation and science in the submitted posters was high, and the enthusiasm of the presenters was refreshing. The winning posters had clean layouts that told a scientific story concisely through an effective combination of text and graphics. All the awardees displayed a clear grasp of their work and could answer both simple and complex questions well. Winners were:

Nicole Webb, Christina Bourne, Paul Hubbard and Ty Gould

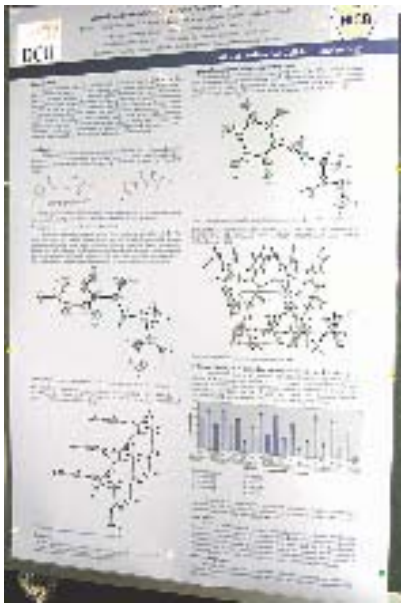
Christina R. Bourne (PP003): **Can Molecular Packing in Protein Crystals Imitate Biology? Frankie Andersen** (PP022): **Fluorobenzoyl Amino Acid and Dipeptide Esters; Paul Hubbard** (PPX054): **Structure and Catalytic Mechanism of Bacterial 2,4-Dienoyl CoA Reductase; Nicole A. Webb** (PP093): **Crystal Structure of a Tetrameric GDP-D-mannose 4,6 dehydratase from a GDP-D-rhamnose Biosynthetic Pathway and Ty Gould** (PPX215): **Quorum Sensing Signal Generation by the AHL Synthase LasI in *Pseudomonas aeruginosa* Pathogenesis.**

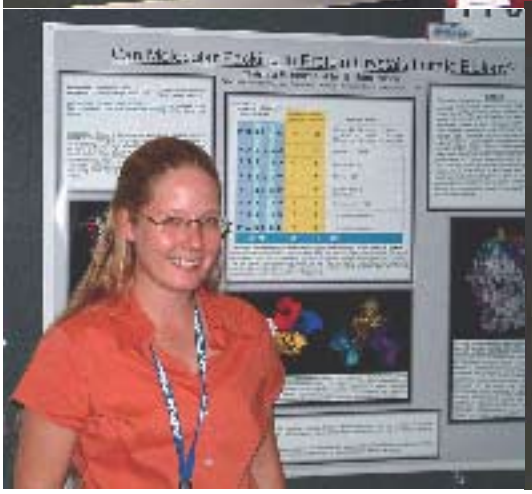
Judges were: ***Frederick Hollander, Chair, Larry Falvello, Christer Aakeroy, Chuck Campana, Fred Wireko, Frank Rotella, Joel Oliver and Tim Mueser***

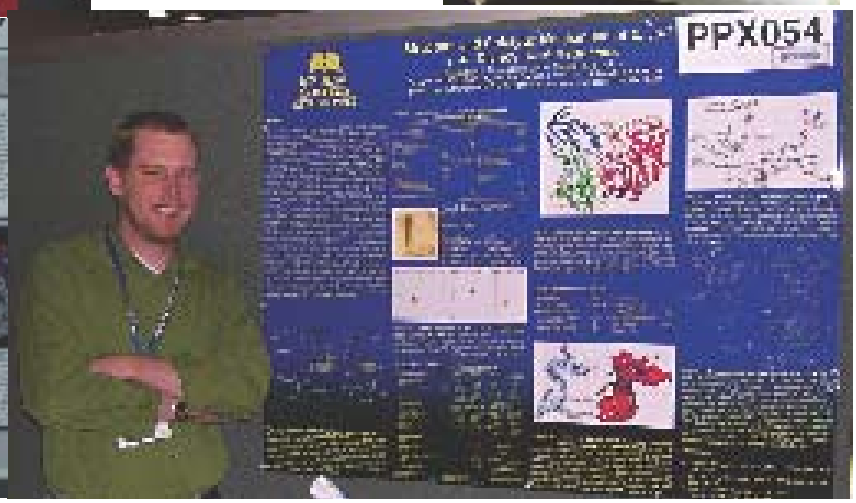


Frankie Anderson. His poster PP022, is at right.

Nicole Webb is at left, and Christina Bourne and Paul Hubbard are below. Ty Gould and his poster are on page opposite.



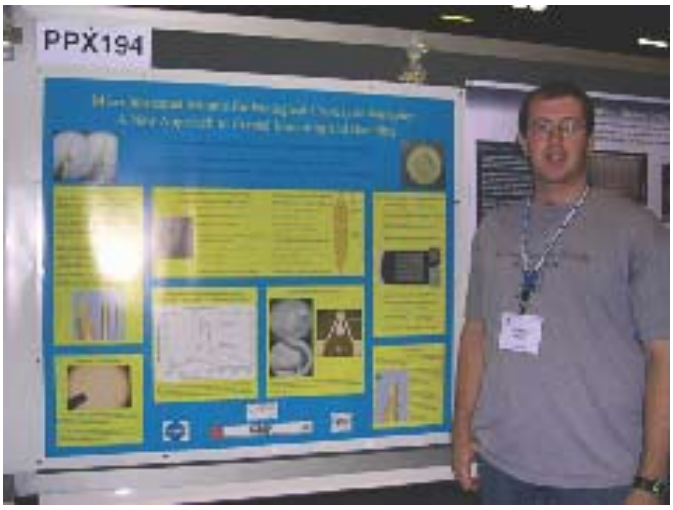




Oxford Cryosystems Low Temperature Prize

The 2003 Oxford Low Temperature Prize was awarded to **Zachary Stum** from Cornell University for PPX194, **Microfabricated Mounts for Microcrystal Cryocrystallography: A New Approach to Crystal Mounting.** This poster described a photolithographic technique for the microfabrication of polyimide mounts which are customizable for crystals ranging from 10 to 100 microns. Although the mounts as fabricated are flat and "floppy", they become quite rigid when curved around a cylindrical base and placed in the low temperature stream. Unlike the loops which are commonly used today, the polyimide mounts do not vibrate when placed in a low-temperature stream. In addition, the excess solution surrounding the crystal is easily wicked away. This, along with the low scattering from the polyimide itself, reduces the amount of background scattering. These mounts seem destined to replace loops.

The committee of judges (Richard Harlow, Chair, Gary Newton, Curt Haltiwanger, Mark Mashuta, and Ewa Skrzypczak-Jankun) had a difficult time selecting a winner, in part because the guidelines for the prize are quite liberal. For the benefit of both future judges and candidates, it should be said that this year's committee decided to down-weight posters where the use of low-temperature was considered standard, such as for routine determination of crystal structure. Instead they focused on posters where LT played a more crucial role in the research, or, as in the case of this year's winner, when the research was likely to strongly impact the use of LT devices. There were two posters which fit the former condition that deserve honorable mention. First, the study of **Mark J. van der Woerd**: PX157, **Perfectly Cold Crystals: What Happens When They Are X-Rayed?** Mark optimized the crystal growth conditions for xylose isomerase to produce crystals that suffered only minimal radiation damage, and then studied the effects of radiation damage as a function of exposure time. Second, **Oleg Borbulevych**, PX198, **X-Ray Structural Studies of Soybean Lipoxygenase-3 at Ambient and 93K Temperatures at 2.0 Å Resolution,** determined that the "pocket" associated with the LT structure is quite different (25% smaller) from that of the room-temperature (in vivo) structure as a result of phase change on cooling. This should serve as a warning to anyone attempting to model the active site using only the LT structure.



Zachary Stum with his prize-winning poster

Three others deserve an honorable mention for the science presented even though the use of LT devices was considered routine. **Karen Knaus**' poster, PPX041, **Crystallographic Studies of the Human Prion Protein**, presented structural results for both the α-helical form and the β-sheet form which the authors propose is responsible for neurodegenerative diseases. **Brad Bennett,** PPX188, **High Resolution X-Ray and Neutron Diffraction Studies of Dihydrofolate Reductase from *E. coli,*** has developed a pathway to produce a perdeuterated enzyme, crystals of which will be usable in a neutron diffraction experiment to pinpoint the origin and pathway of the catalytically relevant protons. **Ty Gould,** PPX215, **Quorum Sensing Signal Generation by the AHL Synthsase LasI in *Pseudomonas aeruginosa* Pathogenesis**, has made extensive use of crystal engineering, mutagensis and mass spectroscopy (for analysis of reaction products) to determine the structures and catalysis of the very complex LasI protein.

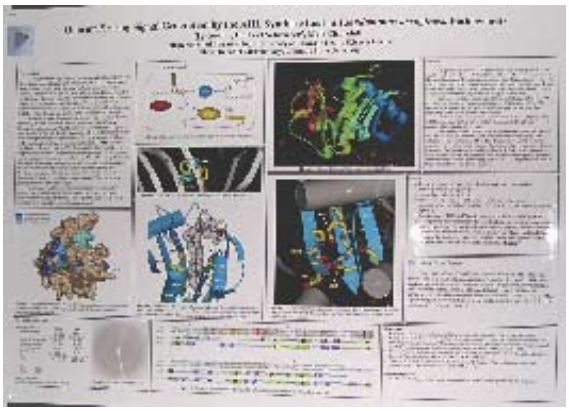
Richard Harlow

First Protein Data Bank Poster Prize

The first-ever PDB Poster Prize was awarded at the ACA meeting to **Ty Gould** for the poster PPX215: **Quorum Sensing Signal Generation by the AHL Synthsase LasI in *Pseudomonas aeruginosa* Pathogenesis**, T.A. Gould, R.C. Murphy, H.P. Schweizer, and M.E.A. Churchill.

A runner-up award was made to **Paul Hubbard** for PPX054: **Structure and Catalytic Mechanism of Bacterial 2, 4 - Dienoyl CoA Reductase**, P. Hubbard, Xiquan Liang, Horst Schulz, and Jung-Ja Kim.

Special thanks to the PDB Poster Prize Committee members Vivien Yee (Chair), Victor Young, Tom Koetzle, Sylvie Doublie, Marvin L. Hackert, and the committee's organizer, Jeanette Krause Bauer.



Ty Gould and his prize-winning poster.

Editor's note: Both Ty and Paul Hubbard won Pauling Prizes as well. See Paul's poster , opposite page.

Call for Nominations for the Wood Award

The Elizabeth Armstrong Wood Science Writing Award is intended to honor people who excel at bringing science to the attention of a wider audience. Successful nominees need not be crystallographers or scientists, and "writing" could be broadly interpreted to include artistic efforts, museum displays, etc.

The award was established in 1997 to honor Betty Wood, who was a crystallographer at Bell Labs until her retirement, an ACA past president (1957), and the author of "*Crystals and Light*," and "*Science From Your Airplane Window.*"

Previous winners include Roald Hoffmann of Cornell, Robert Hazen of the Carnegie Institution in Washington, DC, Robert A. Weinberg of MIT, K.C. Cole, *L.A.Times* Science Writer, and Ira Flatow, who hosts NPR's "*Talk of the Nation, Science Friday*." Nominations should be sent to the ACA office, HWI, 73 High Street, Buffalo, NY 14203-0906 (email **marcia@hwi.buffalo.edu**.)

International Young Chemistry Writer of the Year Award 2003

Are you 16 - 30? Do you want a chance to win $2500 plus an iPAQ Pocket PC? Why not try your hand at writing a feature length article, of between 1000—2000 words, on a chemistry-related topic of interest. Entries can be submitted until 28 November 2003.

The website to find out more and to enter the competition is at: **http://www.chemweb.com/youngwriter**

L'OREAL Art-in-Science Prize

We are pleased to invite ACA members to enter the ***L'OREAL Art and Science of Color*** competition. Entries are welcomed regardless of age or nationality. Prizes are presented for particular pieces of work that have successfully achieved a fresh and original meeting between science and art in color. Entries can be a single work of art, a research paper, or a series of artworks or research papers that have been produced under the same subject or project. Other pieces of work can be attached to the main artwork or research paper as related reference material. The Gold Prize is presented to one person or one group and carries with it an award of Euro 30,000. The Silver Prize is presented to one person or one group and carries with it an award of Euro 20,000. The Bronze Prize is presented to one person or one group and carries with it an award of Euro 10,000. All winners will be invited to the award ceremony to be held in the autumn of 2004 in Tokyo.

Send materials to our Foundation in Japan. The deadline for 2004 entries has not been set yet but will be around the end of March, 2004. For additional information and to see examples of previous winners see: **http://www.art-and-science.com/** or email **lasf@gol.com.**

Yukiko Watanabe, L'OREAL Art & Science Foundation

Call for Nominations for the Shull Prize

The ***Neutron Scattering Society of America*** is requesting nominations for the **Clifford G. Shull Prize in Neutron Science.** The prize is being given to recognize outstanding research in neutron science and leadership promoting the North American neutron scattering community in honor of Clifford G. Shull, who received the Nobel Prize in 1994 with Bert Brockhouse for seminal developments in the field of neutron science. More information is available at: **http://www.neutronscattering.org/ShullPrize/ShullPrizeAnnouncement.htm.**

AIP State Department Science Fellowships

This fellowship program represents an opportunity for scientists to make a unique contribution to the nation's foreign policy. AIP will sponsor one fellow annually to spend a year working in a bureau or office of the State Department, providing scientific and technical expertise to the Department while becoming actively and directly involved in the foreign policy process.

Fellows are required to be US citizens and members of at least one of the 10 AIP Member Societies at the time of application. Qualifications needed include a Ph.D. in physics or closely related field, or equivalent research experience. Applicants should possess interest or experience in scientific or technical aspects of foreign policy. Applications should consist of a letter of intent, a two-page resume, and three letters of reference. Please visit **http://www.aip.org/mgr/sdf.html** for more details. All application materials must be postmarked by November 1, 2003 and sent to: AIP State Dept Science Fellowship, American Institute of Physics, ATTN: Audrey Leath, One Physics Ellipse, College Park, MD 20740-3843. For additional information or questions, please contact Audrey Leath at **aleath@aip.org** or (301) 209-3094.

Flory Gonzalez, Program Coordinator, AIP

Reminder: Please VOTE!

Please remember to VOTE in ACA Elections! Candidate statements and photos are in the summer *ACA Newsletter*; The deadline for mailing ballots or electronic voting via ACA website is November 15th.

Reminder About Visas

Considering the new regulations since 9/11, it is recommended that applications for visas to the US be made AT LEAST NINE MONTHS before they are needed.

The International Visitors Office (IVO) of the National Academies has launched a new website to provide information on visas for visiting scientists and scholars and advice for organizers of international scientific meetings in the United States. Please see: **http://www.nationalacademies.org/visas.**

ACA Council News

ACA Council typically meets formally three times per year: spring, fall, and just prior to the annual meeting. Thus far in 2003, Council has met twice, on Sunday, May 4th in Chicago (site of the 2004 annual meeting) and on Friday, July 25th in Northern Kentucky/Cincinnati just before the ACA 2003 annual meeting. Council will meet again October 16th in Chicago.

Reviewed at both meetings were the financial status of ACA and ACA membership. Council continues to strive to contain meeting costs and to keep registration fees within reasonable limits. Membership has been constant and Council recognizes the importance and the challenge of continuing to attract student members. Meanwhile, corporate membership is the highest in our history.

At the spring meeting, Council met with the chairs of the Local Organizing Committee for 2004, Bernie Santarsiero and Kark Volz (both at U. Illinois at Chicago), Details of the ACA 2004 annual meeting, to be held at the Hyatt Regency in Chicago, were reviewed and discussed. Planning is well underway and on schedule.

At the summer meeting, Mark Brodsky from the American Institute of Physics (AIP) presented an historical perspective of the ACA joining AIP as a member society, reported on the actions of the AIP executive committee, and offered to work with the ACA in various capacities, including documenting history, public relations, and government relations. Iris Torriani (U. of Campinas, Brazil and IUCr Executive Committee member serving as liaison to the ACA) reported on the activities of Latin American crystallographers. Council continues to support the building of relations with crystallographers in fellow countries in the western hemisphere.

In back, from left: S.N. Rao, David Rose, Douglas Ohlendorf, Ray Davis, Bill Duax. In front: Lisa Keefe, Fran Jurnak, Marcia Evans.

Future meeting sites were discussed. The ACA 2005 annual meeting will be held at the Walt Disney World Swan Hotel in Orlando, FL. Sites under consideration for 2006 include Hawaii, Mexico, Canada, and the western USA. So far, Council is considering sites in the southeastern USA for 2007.

Lisa Keefe

News from Canada

1. There are plans by the Canadian National Committee of the IUCr (CNC) to establish a small poster award for presentations at ACA meetings from Canadian laboratories. Funds for this award will be tax deductible in Canada (unlike contributions to other ACA funds) as they will be administered by the CNC. Members living in Canada will be invited to contribute to this fund in a separate request, hopefully to be mailed as part of the ACA membership renewal package. Details are still being worked out, but keep an eye out for this opportunity!

2. **CanadaQuirks: SARS**

In this item, your correspondent will attempt to clarify Canadian terms, organizations, issues, etc. that might be of interest to the Crystallographic community.

Severe Acute Respiratory Syndrome (SARS) has been wreaking havoc on the Toronto tourism and convention industry since early 2003. The episode has been an interesting case study in how far molecular and structural biology have advanced in recent years. Within weeks of the initial outbreak, the causative coronavirus was identified with fairly high certainty. Two to three weeks later, the genome sequence of the SARS coronavirus was elucidated, independently, by the CDC in Atlanta and the BC Cancer Agency in Vancouver. This led in short order to the analysis of likely proteins expressed by the virus, as well as some initial structural modeling (based on sequence similarity) of the main viral protease. More recently, the structure of the protease (not yet published) has been determined and deposited in the PDB. There are now (within six months) established, funded efforts by several agencies, including CIHR and PENCE (see earlier CanadaQuirks) to understand the molecular aspects, immune response and health care issues related to SARS and other emerging diseases (e.g. West Nile virus).

Economic recovery has been much slower, with millions of dollars lost in reduced tourism and cancelled conferences. Through the efforts of the media, the SARS scare has spread across the country, with tourism down in centers hundreds of kilometers from Toronto. Ironically, SARS turns out to be quite difficult to catch in most instances (apart from a very small number of 'super-carriers'). It requires prolonged, close contact with an infected patient. However, there have been no new cases in Toronto for several months and it's safe to come back! You can probably still get great deals on hotel rooms!

David Rose, Canadian Rep. to ACA Council

ACA Communications Committee Report

The Communications Committee has made some plans that we believe can have an impact on the ACA and the crystallographic community. Here are some of the things we are working on, and a number of possible future activities, to enhance "Communications" both within and outside the crystallographic community:

1. **ACA email list** - An up-to-date email distribution list could be an invaluable means to rapidly communicate among our membership, when needed. We are looking for ways to update and to keep current the ACA email list.

2. **ACA Web Site** - The Committee participated in the implementation of the redesigned ACA web site by providing design opinions and testing features of the redesigned web site prior to final rollout. We now need to work on improving the content of the web site, including:

a. **Membership Communication** - The web site is the primary source of rapid communication among our membership. It allows us to inform the membership of changes to the meeting schedule, and other late breaking news, that the quarterly newsletter cannot communicate. The web site also provides a place for the SIGs and standing committees to have their own websites.

b. **Education Resource** - The website should be a starting point to help educators teach, and students learn, crystallography, either via web- links, or possibly through an ACA sponsored initiative to develop our own teaching tool. We have worked with Howard Jones, of the ICDD, to identify useful crystallographic educational web links and materials that are not yet available from either the ACA or ICDD websites.

Our goal is to make the ACA website the FIRST place one would look for any information about crystallography.

3. **Press Kit** - The Committee continues to explore the development of a "press kit" for distribution to the news organizations (TV, newspapers, etc.) in the local area prior to our annual meeting. Such a kit could contain general information on crystallography and the ACA, including history, and impact on science, and details on the upcoming annual meeting. We should also include an invitation to come to the meeting, and perhaps arrange for an informal press conference or tour of the posters and exhibits.

4. **ACA Newsletter** - We believe the **"Web-Watch"** column in the ACA newsletter is an important activity for the committee. It one of the few places where the general membership can see that we, in fact, exist, and are interested in promoting communications. We are hoping to expand this column to include other activities of the committee. We would also like to add the web-pages mentioned in the column to the workable "Links" in the ACA website.

5. **Membership Input and Involvement** - We are always looking for any comments or suggestions from the general membership. We held our first "open" Communications Committee meeting at the Covington ACA meeting. We hope to make this an annual event.

John Sack, Chair, Jeanette Krause Bauer, Kay Onan, Louis Delbaere

Crystallography Web Watch

So, how many crystallographers does it take to screw in a light bulb? *

This month we decided to have a little fun and look at some humorous crystallography and science sites (with maybe a little education thrown in). Start with some Crystallography Jokes from Yoram A. Puius, **http://www.geocities.com/Athens/Forum/7504/xtaljokes.html**

Q: What's the difference between a crystal structure and a molecular dynamics simulation?
A: About 10 Angstroms r.m.s.

Try your hand at the Escher Web Sketcher at **http://www-sphys.unil.ch/escher/** that allows you to create some patterns using crystallographic symmetry. It also includes some links on M.C. Escher.

Some silly crystallography songs (such as "Solve it for me one more time") are found at **http://www.crystal.chem.ed.ac.uk/sillysong.htm** A bit more educational are the Science Songs at **www.acme.com/jef/science_songs** Do you have small children in your life and do you want them to get interested in science? Here is the website for you. These songs are upbeat and infectious and capture many kinds of science phenomena from the making of silk to the definition of humidity. They were originally on six vinyl albums.

Here is a site where you can learn about snow crystals: **http://www.its.caltech.edu/~atomic/snowcrystals/** and even how to grow them yourself. There are also a number of sites giving recipes for growing crystals of various salts. Two of the more complete sites (including references) are **http://www.seawhy.com/xl.html** and **http://rockhoundingar.com/pebblepups/growcryst.html**.

"Rock Candy" from the "Rock Hounding in Arkansas" website above

And be sure to check out Einstein's brain at **http://hometown.aol.com/dvg2**

Have a favorite web site you would like to see in a future **Crystallography Web Watch** column (and maybe linked on the ACA web site)? If so, send the web address and a short (1 or 2 sentence) description to John Sack (**john.sack@bms.com**).

***The answer to the lightbulb joke is, of course:**
None, crystallographers aren't afraid of the dark.

"Dilute Solution" from the Prickly Mountain Project part of Charlie Carter's Past President's talk at the Awards Banquet

Ronald Emerson Burns, inventor of the Xentronics area detector, died at his home in Cambridge, Massachusetts on Friday, July 25, 2003, of cancer. He was 60. His invention of this accurate computer-based x-ray detector was one of the technological advances necessary to propel x-ray crystallography into the essential tool that it is today in the study of the molecular mechanisms of biology and disease. Burns' invention replaced photographic film and conventional diffractometers with a faster, more accurate, and direct method of recording x-ray data into a computer – similar to replacing a conventional still camera with a digital video camera. High throughput x-ray crystallography, which would be impossible without area detectors, is now one of the most important tools used in cancer research.

Ron Burns (1943–2003)

Ron Burns in the Nicolet Booth at the McMaster ACA meeting, 1986, with his Multiwire Detector, the P4-X1000. Photo by Sue Byram .

Ron Burns developed his advanced detector in the early 1980's. He started the Xentronics firm to manufacture his detector in Cambridge, MA. Xentronics was sold to Nicolet Instruments in Madison, Wisconsin, which later sold the business to Siemens AG, which in turn, sold it to Bruker AXS. The first scientists to use the new detector were two researchers at Harvard University, Professor Stephen Harrison, and the late Professor Don Wiley. Using the technology developed by Burns, Harrison and Wiley examined the ways in which viruses bind to cell surfaces, enabling their entry into the cell. Harrison says "the Xentronics detector changed structural biology in a significant way."

Burns was a graduate of Princeton University. He referred to himself as an engineer. After Princeton, he worked at the High Energy Physics Lab at Harvard, while his spare time was devoted to working on and racing motorcycles. Leaving Harvard with only a mental picture of how his detector would function, he worked on his invention for years in his Cambridge basement, drawing on his mechanical intuition to design and build the tools needed to construct the detector. After successfully marketing the invention, he dedicated what turned out to be his remaining years to becoming an accomplished aerobatic pilot and instructor. Ron Burns is survived by his wife, Janet Burns, his son Jason Burns, and his granddaughter Ripley Burns, all of Cambridge, MA.

Paul Aho, Kevin Cameron, Stephen Harrison, and Michael Blum (From the Boston Sunday Globe, July 27, 2003)

Jim Holden (1929-2003)

James R. Holden, 74, formerly of Adelphi, Md., died Sunday, July 20, 2003, in Brunswick, Maine in a hospital not far from his retirement home which he designed and had built in Phippsburg. His decline in health was sudden, and he died peacefully, surrounded by his immediate family.

He received a bachelor of science and a master's degree from the University of Nebraska and earned a doctorate in chemistry from the University of Iowa under N. C. Baenziger. He was a member of *Phi Beta Kappa, Phi Mu Epsilon, Phi Lambda Upsilon*, and *Sigma Xi* in recognition of his academic accomplishments.

His 33-year professional career was with the Department of the Navy, Naval Surface Warfare Center in White Oak, MD, originally called The Naval Ordnance Laboratory,where he worked in the Energetic Materials Division. He was honored with the Navy's Meritorious Civilian Service Award. Jim Holden was a highly respected scientist and was knowledgeable about many things outside his immediate field of expertise. He stayed out of the limelight at NOL/NSWC, but his steady, insightful advice was often sought by his peers and by NOL management as well.

He published extensively, specializing in the determination of molecular structures by x-ray diffraction and the derivation of relationships between molecular structure and physical and explosive properties of organic compounds. Compounds such as 1,3-Diamino-2,4,6-trinitrobenzene were determined by analysis of Patterson functions, but later he successfully applied direct methods to structure determination. More than 20 polynitro aromatic compounds were determined in his laboratory, and this work led to a publication on the relationship between bond lengths and angles in these compounds. As part of the effort to determine these structures he contributed programs to the XRay/XTAL system being developed at the University of Maryland in that era.

In addition to his structure determination work he contributed to a number of government patents. Then, in more recent times, continuing via the Internet after his retirement from the NSWC, he worked on the *ab initio* prediction of crystal structures of

energetic materials, the MOLPAK and ROTPAK programs, in collaboration with Herman Ammon of the University of Maryland. He remained active in this work until shortly before his final illness. Probably his greatest contribution was his empirical method for estimating densities of organic compounds. This effort was driven by the importance of density in predicting the performance of explosives. Before his work there were just two relatively inferior methods for predicting explosive performance. Charlie Dickinson explained that: "Before this contribution the synthesis guys pretty much worked on instinct." Jim, and his colleague Tom Hall, are the authors of The Navy Explosives Handbook, a compendium that is one of the major national references on explosive properties. In addition to his structure work he also contributed to studies which produced phase diagrams of explosive materials.

Jim was also a wonderful colleague to work with and a very thorough person. John Hoffsommer summed it up this way: "I have known Jim for a little over 44 years and consider him one of the finest human beings I have ever known. Jim was always very patient with me and took me step-by-step through the procedures necessary to make x-ray crystallographic measurements. What a wonderful mentor, teacher and friend Jim was!" This sentiment was reinforced by colleagues Ruth Doherty and Lore Kayser who wrote: "Friends like Jim Holden, very special people, don't come along often in a person's lifetime - so when they do treasure them!"

Survivors include his wife of nearly 45 years, Rachel "Daphne" Blachly Holden; two daughters, Carol Holden of Ann Arbor, MI, and Barbara Holden Newman of Bethesda, MD; and four grandsons. Jim was a caring and loving father and husband and will be sorely missed. His daughter reported that he was also a scientist to the end, signaling with his hands and eyes to ask about the nature of the sickness that took him.

Horst Adolph, Herm Ammon, Charlie Dickinson, Ruth Doherty, John Hoffsommer, Lore Kayser, and Jim Stewart

Elizabeth Holt (1939-2003)

The scientific comunity was shocked at the sudden passing of Dr. Elizabeth (Betsy) Manners Holt on June 9, 2003, in Paris, France. She succumbed after a few days to a seizure of unknown origin. She was on a two-week professional/recreational trip to France and Morocco, where she had joint research projects since 1989 with scientists at the Ecole National Superior de Chemie in Lille, France, and at the Department du Chimie du Solide of Mohammed V-Agdal Universite of Rabat, Morocco.

Betsy was born August 2, 1939, in Pittsburgh, PA, the daughter of Theodore and Helen Manners. Her early education was in the public schools of Pittsburgh. She earned a *cum laude* B.S degree from Smith College in 1961 and a Ph.D. from Brown University, under the guidance of Dr. H. R. Nace, in 1966. She was a Research Associate at the Polytechnik Laereanstalt, Copenhagen, Denmark from 1965-66. For the next three years she worked at the Polytechnic Institute of Brooklyn, New York, and then she moved to the University of Wyoming. In 1978 she moved to the University of Georgia as a Research Associate.

In 1980 Betsy moved to the Chemistry Department at Oklahoma State University where she was promoted to Assistant Professor in 1981 and full Professor in 1987. She taught organic chemistry, inorganic chemistry, freshman chemistry, and x-ray crystallography at OSU and was also Director of the X-ray Analysis Laboratory in the Department of Chemistry. In 1988 she received a Fulbright Foundation Fellowship to do research on the analysis of certain phosphate materials common in Morocco.

Betsy's outstanding teaching ability was rewarded by her selection as the AMOCO Foundation Outstanding Teacher in 1984. She received the Etta Louise Gerry National Award for Women Chemists in1981; the *Phi Eta Sigma* Excellence in Undergraduate Teaching in1993; and was the recipient of the Regents Distinguished Teaching Award in 2001. Betsy mentored 11 Ph.D. students, 5 M.S. students, and 28 undergraduate researchers. She collaborated with many on-campus and off-campus scientists and hosted several visiting scientists and post doctoral researchers in her laboratory. She authored more than 250 publications, and more than 100 papers/posters were presented by Betsy, her collaborators, and her students.

Recently her research focused on the structural and physical properties of fluorescent Cu(I) complexes. Her research elucidated the effects of site symmetry, coordination, and elemental composition, providing a basis for understanding the underlying principles of light emission in these and related compounds. She also utilized *ab initio* calculations to demonstrate how symmetry elements impose forbiddenness on expected emissions while allowing others of higher energy. Work on certain calcium complexes of beta-blockers and allergens helped to illuminate the role of such materials in biological regulations and in the immune response. Betsy's work on crystal engineering of selected phosphate complexes led to a variety of pre-organized structures such as linear chains, layered sheets, etc. The incorporation of transition metal ions into these structures leads to a variety of magnetic couplings whose magnitudes and signs depend upon the geometry of their interactions. Applications derived from this work extend far beyond the phosphate-based materials. Betsy is survived by a daughter and a son.

Neil Purdie, Chair, Oklahoma State Chemistry Department

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

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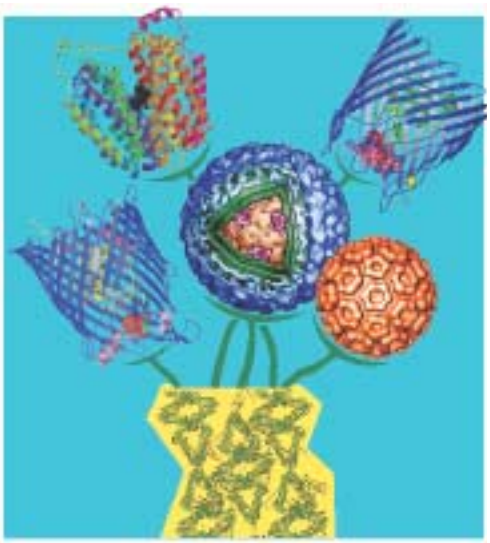


Images from Membrane Protein Structures
at the ACA meeting in Covington, KY

Upper Left: from Jeff Abramson, Imperial College, London, UK. The C154G mutant of LacY, the lactose permease of *E. coli* with a bound high-affinity substrate, ß-D-galactopyranosyl-1-thio-ß-D-galactopyranoside (TDG). LacY is a membrane transport protein belonging to the major facilitator superfamily of transporters.The molecule has N- and C- terminal domains, each with six transmembrane helices, symmetrically positioned within the permease. In the inward-facing conformation, the large internal hydrophilic cavity where the TDG is bound is open to the cytoplasmic side. J.Abramson, I. Smirnova, V. Kasho, G. Verner, H.R. Kaback, and S. Iwata, **Structure and mechanism of the lactose permease of *Escherichia coli,*** *Science* (2003), **301,** 610-615.

Upper right: from Michael Wiener, Univ. of Virginia. The *E. coli* outer membrane cobalamin transporter BtuB. The structure of a ternary complex of BtuB, cyanocobalamin (vitamin B_{12}) and calcium is shown. BtuB, an example of a TonB-dependent outer membrane transporter, consists of a twenty-two stranded ß-barrel domain (shown in blue ribbon) and an amino-terminal hatch domain (shown in green ribbon). The bound cyanocobalamin substrate is shown in space-filling representation, and bound calcium ions are shown as yellow spheres. Calcium, essential for high-affinity substrate binding, causes an ordering of several large extracellular loops of the ß-barrel domain of BtuB. (Figure by David P. Chimento). This structure (as well as SeMet, Apo and Calcium-bound structures) is described in D.P. Chimento, A.K. Mohanty, R.J. Kadner and M.C. Wiener, **Substrate-induced transmembrane signaling in the cobalamin transporter BtuB,** *Nature Structural Biology* (2003) **10**, 394-401. Initial structure determination was by SeMet-SAD with a methionine-substitution construct, the first time such an approach has been used for an integral membrane protein.

Center and center right: from Michael Rossmann, Purdue Univ., West Lafayette, IN: The center blue "flower" with a window is a 22Å resolution structure of Dengue virus. The blue exterior shows the 180 copies of the ectodomain of the E (envelope) glycoprotein. The green represents the lipid bilayer membrane that is transversed by the E and M (membrane) proteins. The red and orange shows the internal nucleocapsid consisting of the about 180 copies of the capsid proteins and the RNA genome. R.J.Kuhn, W. Zhang, M. G. Rossmann, S. V. Pletnev, J. Corver, E. Lenches, C. T. Jones, S.Mukhopadhyay, P. R. Chipman, E. G. Strauss, T. S. Baker, J. H. Strauss, **Structure of Dengue virus: implications for flavivirus organization, maturation, and fusion,** *Cell,* (2002) **108,** 717-725. The figure was prepared by Wei Zhang and is reprinted from *Nature Structural Biology* (2002) **9,** 244, by Tracy Smith, **Does Dengue virus fuse using ß-barrels?**

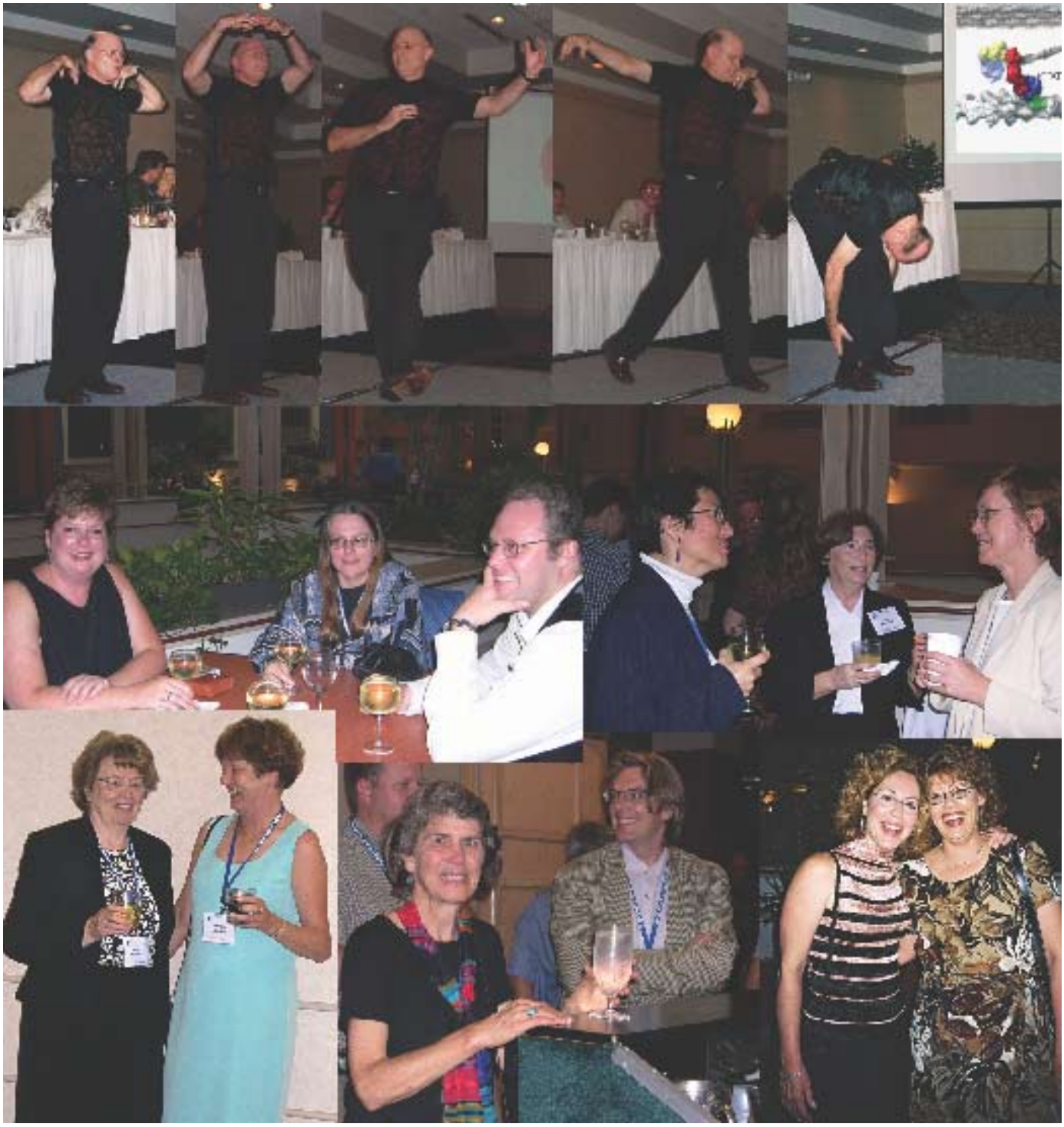
The orange "flower" on the right is the nucleocapsid core of Ross River virus, a member of the alphavirus family. The core consists of 240 copies of the capsid protein in a T=4 quasi symmetry icosahedral arrangment. The figure is reprinted from R.H. Cheng, R.J. Kuhn, N.H. Olson, M.G. Rossmann, H.K. Choi, T.J. Smith, T. S. Baker, **Nucleocapsid and glycoprotein organization in an enveloped virus,** *Cell* (1995) **80**, 621-630.

On yellow "vase" background: from Geoffrey Chang, Scripps Research Inst., Torrey Pines, La Jolla, CA. The crystal packing of MsbA from *E. coli*. The unit cell is superimposed, and this orientation shows the pseudo-222 noncrystallographic symmetry. The figure is reprinted from G. Chang, and C.B. Roth, **Structure of MsbA from *Escherichia coli*: a homolog of the multidrug resistance ATP binding cassette (ABC) transporters**, *Science* (2001), **293**, pp. 1793-1800.

Center left: from Wyatt Yue, Birkbeck College, London, UK. the outer membrane protein FecA bound with iron-free citrate. The mechanism of action proposed by Wyatt Yue and by Sylvestre Grizot and Susan Buchanan who are currently at NIH in Bethesda, MD, involves FecA in three states: unliganded, bound with iron-free citrate as shown, and bound with ferric citrate. The FecA transporter is shown in ribbon representation while iron-free citrate is shown in sphere representation (*Journal of Molecular Biology,* in press).

Editor's note: see also the session report on p 43.

Newport Aquarium photos from Ross Doyle & Victor Young



Scenes from the annual Awards Banquet:

Across the top, Charlie Carter giving his Past-President's address (the choreographed part in which he imitated a favorite structure, not the autobiographical part reminiscing about his formative years in New England and the Prickly Mountain Project).

Middle, from left: Alicia Beatty, Jeannete Krause Bauer, Allen Oliver, Graciela Diaz de Delgado, Iris Torriani, Elena Kondrashkina.

Below, from left: Jenny Glusker and Penny Codding; Martha Teeter, Simon Billinge; and Marcia Evans and Patti Coley

Note: some of Charlie's "Prickly Mountain Project" slides were used as space-fillers in this issue. See pages 21, 35, and 44.

Annual ACA Meeting - Covington, KY, July 26-31, 2003

Highlights of the meeting included the presentations of the **Martin J. Buerger Award** to **Jim Ibers** and the **Bertram E. Warren Diffraction Physics Award** to **Takeshi Egami** (*see page 13*). The ***Transactions* Symposium**, on ***Biological Neutron Diffraction*** was organized by Gerard Bunick and Leif Hanson; and there were two special symposia: ***Time Resolved Diffraction in Chemistry and Biology***, organized by Philip Coppens and Keith Moffat, and ***Future Strategies for Successful Crystallographic Computing***, organized by Ross Angel and David Watkin. Sessions were organized to honor the Buerger and Warren Award recipients and there was also a special session to honor **Julia Chan**, the first recipient of the **Margaret C. Etter Career Award** *(see pages 13-15 for the Etter Career and Student Lecturer Awards, and the 2003 Pauling, Oxford, and PDB Poster Prize winners.)* Reports of many of the sessions are on following pages, but the ***Membrane Protein Structures*** session organized by Johann Deisenhofer and Douglas Rees deserves special mention because it was the inspiration for the cover of this *Newsletter* (*see pages 27 and 43*). Congratulations to Program Chair Jeanette Krause Bauer and the other members of her program committee for organizing an excellent program!

Local Chair Bobby Barnett and Program Chair Jeanette Krause Bauer

The Northern Kentucky Convention Center was a very pleasant and comfortable fit for us; hotels and restaurants were conveniently located, and there is ample photographic evidence (special thanks to Victor Young, Ross Doyle, and Judy Flippen-Anderson) - that the social program was a lot of fun. Local Chair Bobby Barnett and the members of his local committee, particularly food and entertainment coordinator Ann Wolff, did a wonderful job with the opening reception at the Newport Aquarium, the Awards Banquet, and the final evening dinner cruise on the Ohio river. The YSSIG mixer, was a huge success, as was the Mentor/Mentee dinner at Chez Nora.

"Cincinnati twilight" - photo by Ross Doyle

As always, our exhibitors contributed generously and imaginatively to the social scene. The Bruker Riverboat excursion, the Mar-USA evening social at the Strasse House in German Town, and the Rigaku/MSC fun run (across the bridge and around the stadium) were fine examples of their benevolence.

Scenes from the YSSIG mixer at Jack Quinn's Pub, and three examples out of what seemed to be hundreds of "baseball art" outdoor sculptures found everywhere around the city.

It is trivial to state that all reactions in chemistry and biology involve changes in structure at the atomic level, not just quasi-static, time-averaged structures; but the elucidation of these changes in structure poses significant experimental challenges to the crystallographic and structural communities. This Symposium addressed the present state of the art as applied to chemical and biological problems. Speakers provided both overviews of the techniques themselves (including both x-ray and electron scattering, and x-ray spectroscopies as well as chemical and biological crystallography), and numerous examples of recent applications. Speakers ranged from graduate students (**Melanie Saes**, U. Lausanne; **Sonia Larsen**, U. Illinois at Chicago; **Jason Key**, U. Chicago) through post-docs (**Harry Ihee**, U. Chicago), to junior faculty, staff scientists at synchrotron facilities, and finally to grey-headed senior scientists (remaining nameless here). The symposium was sponsored by the Petroleum Research Fund of the ACS, and by the Chem/MatCARS and BioCARS organizations at the Advanced Photon Source. Registration waivers for invited speakers were provided by the ACA. The Symposium brought together scientists from different disciplines using a variety of techniques, which, as became clear during the meeting, nevertheless have many features in common.

Simone Techert (Max Planck Institute, Goettingen), **Lin Chen** (Argonne) and **Melanie Saes** opened the first session with three talks all with strong chemical orientation, covering time-resolved diffraction of organic solids and time-resolved XAFS and x-ray absorption of electron-transferred excited states of transition-metal (Cu(I) and Ru(II)) complexes in solution on timescales ranging from femtoseconds to nanoseconds. In the final part of the session the time-resolved x-ray diffraction facility of Chem/MatCARS at APS was described by **Tim Graber** and the first atomic-resolution experimental results on microsecond-lifetime excited states of a Cu(I) complex after metal-to-ligand charge transfer were reported by **Philip Coppens** (SUNY/Buffalo).

The second chemistry-oriented session covered time-resolved electron diffraction experiments of light-induced processes in solids and solutions (**Ivan Tomov** of the Rentzepis lab, UC Irvine) and femtosecond gas-phase electron diffraction studies of the ring opening of 1,3 cyclohexadiene (**Peter Weber**, Brown Univ.). Weber pointed out that it should be possible to study oriented molecules in the gas-phase

SP02: Future strategies for successful crystallographic computing

It was standing room only throughout the half-day session concerned with the future support of crystallographic software. The first half of the morning was devoted mostly to defining the issues, both old and new. **David Watkin** (Univ. of Oxford) opened the session with a review of the history of crystallographic software development. He particularly contrasted a golden past in which software diversity was maintained by widespread programming skills, public domain distribution, free maintenance, and open cooperation between developers with the gloomy present of market forces not only in commerce but also within universities and government labs. He noted examples of crystallographic software being effectively killed by universities demanding licensing fees and expressed a concern about "creeping entrapment" whereby free software is not maintained because of lack of funding, with the result that the underlying ideas are eventually lost to the community.

The new issue of software patents was reviewed by **Lachlan Cranswick** (Chalk River). He showed that patents on basic concepts such as reflection centering, structure solution and least-squares refinement are now being passed by patent offices leaving the entire community open to legal action. He summarized the potential dangers of such patents and patent actions with the memorable phrase that "we cannot stand on the shoulders of giants if the giants wear spiked shoulder pads." Readers interested in seeing whether they already violate a software patent ***(and that really does mean every single member of the ACA)*** should consult an article at **www.iucr.org/iucr-top/comm/ccom/newsletters/2003jan/** and read Lachlan's review at **www.ccp14.ac.uk/maths/software-patents**. Some of the subsequent discussion focused on the role of gnu software licenses although it was clear that such licenses address issues of copyrights rather than patents. **Carroll Johnson** (Oak Ridge) continued the list of difficulties facing the modern programmer with a synopsis of security issues and the inadequate tools available to address them. A show of hands in the discussion session revealed the seriousness of the situation in that most present knew that their labs had been the victims of hackers and/or viruses, or believed that they may have been and have not yet found out.

Software development and diversity were the themes of the second half of the session. **Brian Toby** of NIST reflected on the life and career of a typical software developer in the US government labs where much of our current crystallographic software started life, but where such development is not directly supported. He felt that software and algorithm developers needed more public recognition by the community, a point that was well-received by the packed audience. And he used the 20 year development history of Rietveld codes as an argument to show that were software to be only developed on a purely commercial basis it would stagnate, as development timescales are far longer than is acceptable for commercial products. **Sue Byram** described strategies at Bruker/Nonius to ensure diversity by pursuing in-house software development in parallel with the integration of software from various other sources into their packages. Oxford Diffraction's **Mathias Meyer** described a slightly different solution to integration of commercial and academic code through offering open-source software and the integration of user's software packages through plug-ins.

con't page 34

SP.02 Crystallographic Computing, con't

Back row, from left: Paul Adams, Sue Byram, Ross Angel, David Watkin, Lachlan Cranswick, Jim Pflugrath, Mathias Meyer; In front: Brian Toby and Carroll Johnson.

Another way of promoting diversity in software is to make it easier for people to program algorithms by providing software "toolboxes." **Paul Adams** (Lawrence Berkeley National Lab) described the development of one such system, *Phenix*, and its associated cctbx toolbox. Subsequent discussion of the project focused on how the development of *Phenix* is supported financially, and whether it would survive in the longer term. Discussion got quite heated over the difference in cost between academic and commercial licenses. David Watkin meanwhile pointed out that a similar toolbox, the Cambridge Crystallographic Subroutine Library (CCSL) had been developed with the same aims more than 20 years ago. A show of hands indicated that only 3 of the 100 or so attendees at the session had heard of it, illustrating that long-term support of such resources for the benefit of the community can clearly be problematic. That show of hands also indicated to your surprised correspondent that he had joined the "older generation"!

The extensive discussions and thought-provoking presentations through the morning boiled these various issues down to software diversity, software support, and the training of programmers. Reassuringly, several speakers and discussion participants felt that there was no shortage of crystallographic programmers and that various methods are available to ensure the continuing development of that work force. Support of software development and maintenance and retention of software diversity are clearly inextricably linked as, in the words of the title of **Joe Pflugrath**'s presentation, "There is no such thing as free software". While there is general agreement that software diversity needs to be maintained, there are clearly differing views as to how this should be ensured or whether a simple evolutionary approach of "survival of the fittest" is to be desired. Distilling the views expressed in the general discussion session, your correspondent believes that a diversity of support mechanisms will ensure a diversity of software. Such support should range from grant-funded software archives and clearing houses such as ccp14, payment of realistic fees for commercial software, and the recognition that grant support is appropriate for both developers in the academic environment and to end-users to enable them to purchase commercial software. And most importantly, as George Sheldrick reminded everyone, the publishing of software notices and descriptions in journals such as *J. Appl. Cryst.*, and the citing of such sources by all those who use the software is essential. With such citations, programmers can justify their existence to supervisors and department chairs, as well as stand a chance of gaining financial support for their efforts from funding agencies. So, everyone left the session more reassured than at the start of the morning, but conscious that much needs to be done to raise the status of crystallographic programming back to where it was several decades ago. After all, without software we would all be using Beevers-Lipson strips!

Ross Angel

AW.01 Warren Award Symposium

Front, from left: Despina Louca, Sossina Haile, Takeshi Egami, Brian Toby, Pencheng Dai; in back: Doug Buttrey, David Rosenfeld, Peter Chupas

An inspiring array of speakers, from around the US and the world, gathered to honor Prof. Takeshi Egami on the occasion of his receipt of the Warren Award. This session was greatly facilitated by the generous support of the Joint Institute for Neutron Science (JINS) and the University of Tennessee. Prof. Egami has a long-standing interest in materials exhibiting structural disorder and a broad spectrum of these was represented in the symposium. Increasingly, advanced functional materials have significant amounts of structural disorder and revealing the beauty and relevance of this complexity is an important goal of research. The materials described in the symposium ranged from synthetic analogs of trans-membrane proteins to bulk metallic glass. Several structural characterization methods were in evidence. The method of atomic pair distribution function (PDF) analysis of x-ray and neutron powder diffraction, which Prof. Egami played a key role in developing, was well represented, but other approaches, including neutron reflectometry, x-ray microtomography and inelastic neutron scattering were described as well. A theme that recurred in many presentations is that it takes more than one experimental method to complete the detailed structural characterization of complex materials.

Another common theme was that those who study these disordered and partially ordered materials are pioneers. **Takashi Egami** in his award lecture outlined the difficulty of getting new techniques and novel ideas accepted, the resistance encountered and

perseverance required before concepts become established. The Rietveld method of structure refinement from powders is a key example. Few people these days who routinely use and rely on this technique remember that, as recently as 15 years ago, results of Rietveld refinement were viewed with suspicion; efforts to broaden the scope of the technique to x-ray powder diffraction and pulsed neutron diffraction were met by derision and opposition. Similar experiences were recounted in other talks. **J. Kent Blasie** (U. Pennsylvania) related how he had been told that the phase problem in reflectometry could not be solved. He then told us how he and his colleagues have solved that problem and are using it to study synthetic analogs of trans-membrane charge transfer proteins. Remarkably, by selective deuteration, it is possible to determine the height of a particular amino acid with precision on the order of 0.1 Å even though the wavelength of the radiation used in this technique is much longer than 1 Å. **John Finney** (University College London) also defied the advice of his learned colleagues that it was hopeless to study the structure of complex liquids. He showed how we can now determine not only the arrangement of solvent molecules around solute molecules, but also their orientation. As a result, completely new insight is being gained into a fundamental problem that has been studied with little progress for more than 100 years: that of salting out of amphiphiles from solution. **Shenda Baker** (Harvey Mudd) also described the patience and persistence required when confronting theorists with convincing data that do not agree with their theoretical predictions. Novel pioneering techniques only become fully mature when it is possible to know their limitations and **Brian Toby** (NIST) told us how to estimate the standard uncertainty, and therefore the degree of confidence we can have in structural parameters refined from the PDF, an important milestone in the coming-of-age of the PDF method. Novel applications of the adolescent PDF technique to study strain in bulk metallic glasses (**Ersan Üstündag**, Caltech) and fast, time resolved, measurements of catalytic ceria undergoing reduction and oxidation *in-situ* (**Peter Chupas**, SUNY-Stony Brook) showed imaginative extensions of the technique.

Remarkably, by selective deuteration, it is possible to determine the height of a particular amino acid with precision on the order of 0.1 Å even though the wavelength of the radiation used in this technique is much longer than 1 Å.

Complex electronic oxides continue to surprise and confound us. Takeshi Egami's early insight that the atomic structure is an important determinant of their properties is only now being confirmed by results from multiple techniques. **Despina Louca** (U. Virginia) and **Pengcheng Dai** (U. Tennessee) gave fascinating insights into the coupled lattice and electronic systems of these materials. **Branton Campbell** (U. Utah) described an elegant solution that, together with **Sunhil Sinha** (U. California, San Diego), solved the problem of extracting microscopic information about Jahn-Teller defects in electronic manganites from x-ray diffuse scattering measurements. This approach force-coupled the defect to the elastic medium of the material, allowing quantitative microscopic information to be deduced from the Huang scattering signal. This creative and innovative solution caught the pioneering spirit of the session. Also ingenious is the use of Pauling's ice rules to calculate configurational entropy of disordered hydrogen bonds in hydrogen sulphate protonic conductors (**Sossina Haile**, Caltech). **Doug Buttrey** (U. Delaware) revealed how to find beauty and fine dining starting from a "dog's breakfast", the description coined for his chemically complex but exquisitely catalytically important, mixed phase molybdenum oxides. His group combined electron microscopy and neutron and synchrotron powder diffraction for a multi-technique structure solution tour-de-force. **Brent Fultz** (Caltech) presented his struggle, ultimately successful, to extract site-specific structural information using Mossbauer scattering to perform diffraction.

The session had a festive spirit about it because it was a celebration of years of innovation from the group of Prof. Egami. **Wojtek Dmowski** (U. Tennessee) related some adventures from PDF-land saluting a DEC microVAX, named PDFVAX on which much of the early work in the Egami group was carried out. The session closed with some delving by **Simon Billinge** (Michigan State U.) into Takeshi's early life which revealed compelling evidence that he is closely related to Shigeru Egami, a pioneer of karate in the early part of the last century. This was then followed with a presentation on how the Billinge group is extending the PDF technique in many directions, including nanostructure studies.

Simon Billinge

"*Radial Symmetry*" from Charlie Carter's *Prickly Mountain Project* talk (see p 28).

AW.03 Margaret C. Etter Award Session

Below, ACA President presenting Julia Chan with her Career Award. (see p 13).

1.01: Difficult Structures
(a.k.a. high hanging fruit)

In a brief introduction the session chair reflected on the fact that in spite of the amazing improvements in hardware, software and methodology, difficult structures are likely to remain with us for some time to come. This was illustrated beautifully in the following six presentations that showed problems and solutions in many of the steps needed to obtain a crystal structure. **Song Tan** opened with a very stimulating and practical presentation on the need for co-expression systems to study larger protein complexes. He showed several examples of hetero-multimers in such intimate embrace that it was clearly impossible for them to be produced in isolation. One approach is to produce each monomer as inclusion bodies and then form the complex by refolding the mixture. The bulk of the presentation was, however, devoted to a polycistronic *E. coli* expression vector created in Tan's laboratory and the various hetero-multimeric eukaryotic protein complex structures that were solved using the system.

Travis Gallagher surprised us all by stating that one of his problems was too many crystals. About 25% of Hampton Screen 1 gave crystals of his alanine dehydrogenase but, alas, none were good diffractors. A major dilemma was to properly estimate the suitability of a crystal; underestimation results in time wasted optimizing crystallization conditions, whereas overestimation results in time wasted on unsuccessful phasing attempts. One $P2_12_12_1$ crystal form had an NCS 2-fold parallel to a crystallographic 2-fold and addition of Sm or Ir caused a 6 Å shift resulting in a $P2_12_12$ crystal form with a two times smaller unit cell. The anomalous signal of these derivatives combined with a better native crystal form, grown by accident from a drop lacking mother liquor ("precipitant-free crystallization"), led to a successful structure determination. One interesting structural feature was the observation of Asp/Glu residues interacting with each other in crystal contacts. These crystals were grown by a pH shift from 5.5 to 4.0 and at the lower pH dicarboxylates may actually be able to form a stabilizing hydrogen-bonded interaction.

Urszula Derewenda, did not "suffer from" too many crystals of LcrV, a virulence factor of *Yersinia pestis*. Instead she resorted to mutating clusters of hydrophilic residues, especially ones including lysine, to alanine residues in an attempt to reduce loss of entropy upon crystal formation for these flexible side chains. Interestingly, four out of five mutants now formed crystals. Selenium atom positions were readily determined by SHELXD from 3-wavelength MAD data. However, SHARP refinement failed initially but was made to work by first refining in MLPHARE followed by multiple SHARP runs refining one variable at a time. One interesting though not really understood observation, was that significantly better results were obtained after the MAD data was rescaled against the peak data set. In the end the speaker was rewarded for her perseverance by finding a new protein fold.

Front row, from left: Vivien Yee, Tina Bakolitsa, Urszula Derewenda. From left in back: Travis Gallagher, Song Tan, Fred Vellieux, Bart Hazes, Debanu Das.

Debanu Das shared his adventure with the Moloney murine leukemia virus reverse transcriptase:DNA complex. Crystallization proved again very challenging and required N-terminal truncation, mutation of a single residue in a hydrophobic stretch to remove dependence on detergents during protein purification, and testing of over 25 oligonucleotides. The crystals were extremely small and data could not be collected without synchrotron sources. Since MR could place only the N-terminal domain (~35 % of the whole molecule), the structure was determined using combined phases provided by MR, U, Au and Se (with two extra methionines introduced into the N-terminal domain). After solvent flattening the density finally allowed the structure to be built to 3.0 Å resolution, revealing striking structural differences when compared to the functionally related HIV-1 RT protein. **Tina Bakolitsa** described a tough SeMet structure determination of the vinculin head domain. Crystals were highly mosaic but improved upon cryo-annealing. A long cell edge, weak diffraction, and low crystal symmetry complicated data collection, especially for the SeMet crystals, which were very radiation sensitive. Global scaling/Shake-and-Bake and local scaling/SOLVE failed, while local scaling/XPREP+SHELX succeeded in locating a majority of the Se positions using 4.5 Å resolution data. Two-wavelength (inflection and high energy remote) SeMet MAD phases were used to place MR models of the N- and C-terminal domains; Se sites and secondary structure prediction aided model tracing. Upon rigid body refinement of helices and phase extension to 3.3 Å resolution, difference density identified side chains, and SIRAS with Pt and Hg derivatives resolved sequence ambiguities. CNS refinement is underway with H-bond restraints and sharpened data.

Fred Vellieux closed the session with his tale of trypanosomal pyruvate phosphate dikinase. Since only one protein batch yielded crystals, and all crystals were consumed in obtaining a single native dataset, MR with a bacterial homolog was the only available method for structure determination. Using the complete bacterial structure as the search model was unsuccessful and the structure was therefore solved stepwise. First the C-terminal domain was placed and fixed after which the C-terminal fragment of the N-terminal domain could be located followed by the N-terminal fragment of the N-terminal domain. However, the phospho-His domain could not be placed by traditional MR but there was some discontinuous density for it. To overcome this, Fred set the density within the mask encompassing the known parts of the model to zero ("protein flattening"). This procedure greatly cleans up the corresponding Patterson map and MR against the structure factors obtained after map inversion detected the missing domain as the top peak in a rotation search, and the second peak in the ensuing translation search.

Vivien Yee and Bart Hazes

Macromolecular Posters: Anomalous Scattering

Several poster presentations at the 2003 ACA meeting pushed the boundaries of using anomalous scattering signals from sulfur, selenium, and other atoms in macromolecular crystal structure determinations. Their subject matter ranged from the development of new techniques to solving and refining new structures. An ultimate goal of these posters was to allow the minimum amount of diffraction data necessary to be collected in an automated way; that is, with fewer and weaker anomalous scatterers, less data redundancy, collected at fewer wavelengths with fewer photons. Or, in other words, the goal is to make macromolecular structure determination as routine as that for small molecule crystals.

In the realm of new techniques, **Zheng-Qing Fu** et al (U. Georgia, P031) devised the ratio Ras to help answer the questions *"Is the data quality still improving by collecting more data?"* and *"Is the data collected sufficient to solve the structure?"* They argued that Rsym, $\langle I/\sigma I \rangle$ and $\langle \Delta I/\sigma I \rangle$ are not objective and accurate enough measures to inform the experimentalist of the anomalous scattering signal/noise ratio. As a better measure of anomalous-signal-to-noise, they proposed the ratio Ras = $\Delta a/\Delta c$, where Δa is the $\langle |I^+ - I^-| \rangle$ for acentric reflections and Δc similarly for centric reflections.

Anita Coetzee et al (Bruker Nonius, BV, P102) coined the phrase "serendipitous redundancy" to stress that multiple measurements of the same reflection in the same orientation does not provide the benefits of "true redundancy," that is, multiple measurements of the same reflection with different paths through the crystal and/or symmetry equivalent reflections. They were able to solve the thaumatin crystal structure from sulfur SAD data collected in 9 different scans, aided by intelligent strategy software, on a home lab microfocus copper rotating anode.

Cheng Yang et al (Rigaku/MSC, P124) reported on the use of chromium radiation in the home lab to phase the crystal structures of thaumatin, trypsin, glucose isomerase, proteinase K, and a few proprietary proteins. The $\Delta f''$ for calcium, sulfur, selenium, and other elements is significantly increased at the 2.29 Å wavelength relative to copper radiation at 1.54 Å. They were able to increase the flux on the crystal by using a microfocus rotating anode generator coupled with a multilayer optic. The absorption problem of the soft x-rays was reduced with a helium beampath. Neither high resolution nor high redundancy data were required to achieve these results. For tetragonal thaumatin, a single 45° scan of data of comparatively low redundancy was sufficient to phase the observed structure factors. Another benefit was the ability to resolve unit cell axes of over 600 Å in a home lab experiment.

Qun Liu et al (Cornell U. and U. of Science and Technology of China, Hefei, P153) proposed a SAD phasing protocol for high-throughput structure determination. Their test case was a protein with co-crystallized copper measured at the copper Kα-edge to 1.5 Å resolution. They solved the structure using direct methods and were able to determine the correct handedness of the structure from only the copper substructure.

Jun Wang and Steven Ealick (Cornell U., P187) showed that diffraction data collected at 1.5 Å wavelength from cubic insulin crystals could be phased from the sulfur anomalous scattering signal with less than 5-fold redundancy, if one took care to apply different corrections to the estimated sigmas of measurements from different images.

How many selenium atoms does your protein need to do successful SAD phasing? **Rong Guang Zhang** et al (Argonne National Lab, P207) demonstrated that you need just one for a 32-kDa protein. The protein in question was a hypothetical protein from *Staphylococcus aureus*; SAD data to 1.7 Å resolution. Diffraction data were collected at the peak wavelength of the selenium K-edge in 15 minutes using the insertion-device beamline of the Structural Biology Center at Argonne's Advanced Photon Source.

As weak anomalous scattering signals are exploited more and more routinely because of the ideas presented in these posters and in the talks, dare we write that perhaps the Service Crystallography SIG will be dominated by macromolecular crystallographers in 5 years?

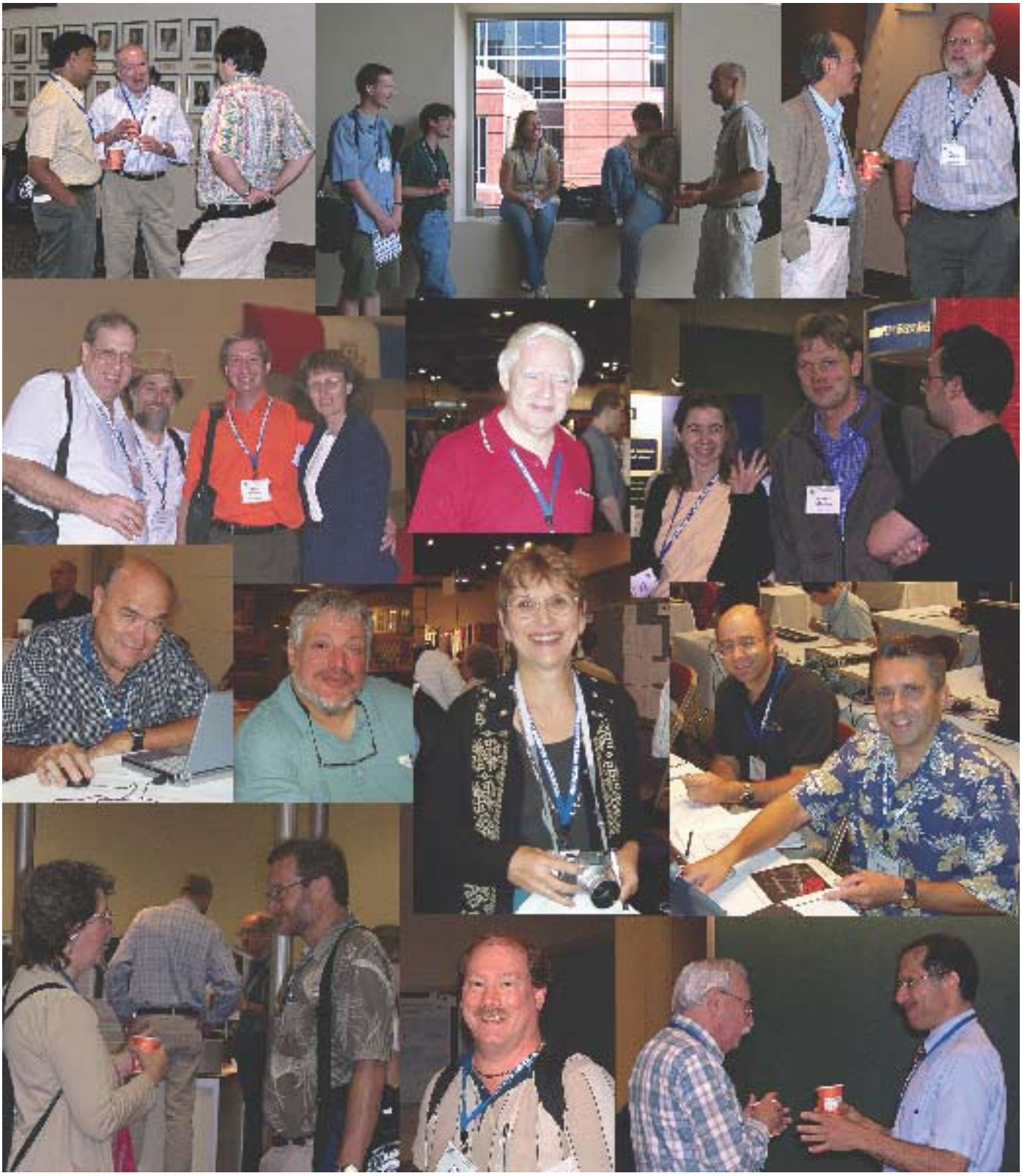
Jim Pflugrath and Frank Rotella

1.02: Computational Methods

The Sunday afternoon session hosted seven presentations and was very well attended. Computational aspects of structure determinations were addressed from crystallization to the final validated structure by giving some recent highlights in each field. Topics included evaluation of crystallization experiments, structure solution, model building, structure validation, and the comparison of multiple structures.

Julie Wilson (York Structural Biology Laboratory at U.York) presented a very interesting talk on the algorithm that she is developing in order to identify crystals in vapor diffusion experiments by automatic evaluation of images. The images are pre-processed to isolate the drops and enhance crystal-like objects. Based upon a number of image features, images are classified as diffraction quality crystals, poorer quality crystals, or precipitate. **Airlie McCoy** (Cambridge Institute for Medical Research), Welcome Trust described a new program, Phaser, which incorporates maximum likelihood into the rotation and translation functions. Previous experience has shown that maximum likelihood rotation and translation targets are more sensitive to the correct solution than traditional methods. Series approximations are used to derive a fast maximum likelihood molecular replacement target that can be computed by an FFT. Several examples were presented that illustrated the advantages of Phaser. **Ralf Grosse-Kunstleve** of the Lawrence Berkeley National Laboratory described the Phenix substructure search procedure. The method is designed to improve heavy atom or substructure search techniques through the integration of Patterson functions, fast translation functions, Sayre squaring, and a random omit procedure. Both memory requirements and computational time are significantly reduced. The program is implemented in the Python scripting language making extensive usage of the newly developed cctbx crystallographic computing toolkit, which is developed by the Phenix team.

con't page 39



At top, from left: Ravi Kurumbail, Hans Deisenhofer and Fred Vellieux; Scott Reid, Alex Singer, Jill Chrencik, Paul Shaffer & Eric Wise; Wah Chiu and Wayne Anderson.

Next below: Leif Hanson, Andy Howard, Marc Whitlow & Sue Byram; George Sheldrick; Katusa Breje, Thomas Schneider and Tassos Perrakis.

Next, from left: John Huffman; Frank Rotella; Judy Flippen-Anderson; Jim Fettinger and Joe Ziller.

Bottom: Paula Fitzgerald and Rick Bott; Victor Young; Abe Clearfield and Larry Falvello.

1.02: Computational Methods, con't

Serge Cohen (Netherlands Cancer Institute) presented some recent developments in the ARP/wARP software. The aim of these procedures is to improve the completeness of auto-build models by improved sequence assignment procedures that handle non-crystallographic symmetry in an efficient manner, side chain rotamer building and building of flexible loops. **John Badger** (Structural GenomiX, Inc.) presented the results of validation of structures from their own database. Software has been developed to automatically refit incorrect fragments or substrates. In cases where the structure is inaccurate, refitting has been shown to be comparable to simulated annealing. The automated procedures that have been employed produce up to 90% of the final structure prior to manual model building. **John Westbrook** (PDB, Rutgers), described a set of software tools that can be downloaded and used to validate structure depositions. In addition, programs are available that can read the output from most refinement packages and generate the required information for a deposition, resulting in minimal effort in the preparation of a deposition. The suggestion was made that PDB deposition reports could be electronically packaged so that they could accompany a manuscript through the peer review process. **Thomas R. Schneider** (U. Gottingen) described a very elegant genetic algorithm for the comparison of multiple structural models. Following normalization using estimated standard deviations, difference distance matrices are calculated for multiple structures as a means to identify those portions of the structures that are similar and those that contain significant changes in conformation. Thus, the method requires no prior assumptions about structural similarities and permits an objective comparison of multiple structures. Several examples were illustrated, demonstrating the utility of the procedure.

Software has been developed to automatically refit incorrect fragments or substrates. In cases where the structure is inaccurate, refitting has been shown to be comparable to simulated annealing.

Anastassis Perrakis and G. David Smith

Posters: Protein Structures with Ligands

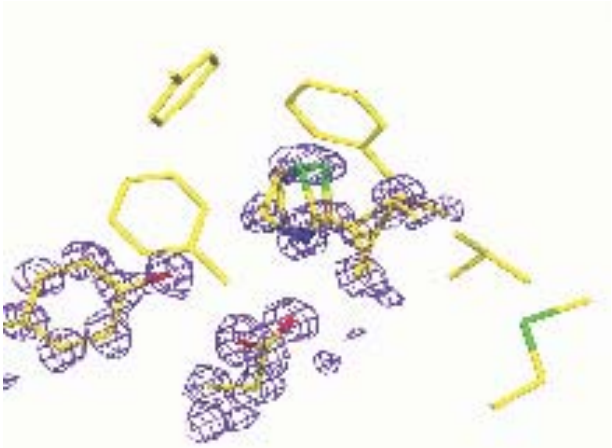
Two interesting posters presented novel applications of macromolecular structure determination. P053 by **V. Cody, J. R. Luft**, and **W. Pangborn** presented 1.9Å & 2.3Å resolution complexes of human and bacterial dihydrofolate reductase with a novel tetrahydroquinazoline antifolate. The enzyme was crystallized with a racemic mixture of 6R- and 6S-2,4-diamino-6-(1-indolinomethyl)-5,6,7,8-tetrahydroquinazoline. The structure of the human ternary complex (with NADPH) showed that the enzyme resolved the racemic mixture, binding the 6S-equitorial enantiomer preferentially. The authors are among the first to use macromolecular crystallography to determine which enantiomer is active.

P088 by **Q. Zou, T. Hurley**, and **M. Novotny** presented a 1.55Å resolution structure of mouse major urinary protein-4 (MUP4) one of a number of MUPs that help transport various mouse pheromones. The novel application of this structure was the revelation that a flavoring molecule was bound to MUP4; because the work was done at high resolution, the molecule could be identified as 2-ethyl-1-hexanol thereby demonstrating an analytical application of structure determination. The overall structure of MUP4 does not differ substantially from that of MUP1 except that residue 136, a glutamate in MUP4, was found to undergo a conformational change to bind to different ligands. In contrast to the enantiomer specificity of DHFR found in P053, MUP4 was found to bind to both R and S forms of the pheromone.

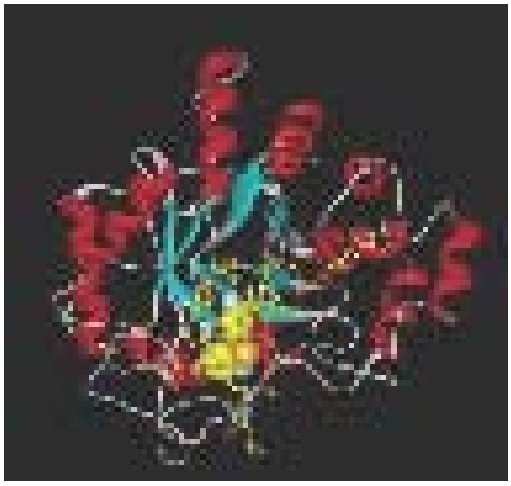
The conformational flexibility of protein structures, particularly in formation of complexes with ligands, is another theme seen in several posters. P216 by **C. Lautenschlager** and **J. Clardy** presented structures at 1.9Å and 2.0Å of complexes of *B. mori* pheromone binding proteins (PBP) with iodohexadecane and with bell pepper odorant. The conformation of PBP was similar to that observed in the PBP and sex pheromone bombykol complex; however, the conformational change on binding was more pronounced than for the mouse pheromones presented in P088. The structure of unliganded *B. mori* PBP was significantly changed from that of the complex – the C-terminal region formed a helix that occupied the binding pocket. Another example of conformational change was the structural effects of leukemia drug Ara-C on human topoisomerase I DNA complex (P081 by **J. Chrencik**). Incorporation of the drug results in DNA opening up to bind the drug plus a one base pair shift downstream. Drug binding causes shifts as large as 8.7Å in the position of some residues and changes in the enzyme 13 Å away from the drug binding site.

The structural results presented in these posters showed the power of high resolution work to determine enantiomer specificity and the identity of unsuspected ligands and showed that structural work is essential to understanding the unpredictable conformational effects of complex formation.

Penelope Codding



From Qin Zou: MUP4 complexed with the mouse pheromone (SBT) at 0.96 Å.



From Andrzej Joachimiak, (fig. prepared by Alberto Podjarny): an atomic resolution (0.9 Å) experimental map from a MAD experiment using a SeMet labeled crystal of human aldose reductase. (Data collected at SBC 19 ID beamline at APS. (Podjarny, A., Schneider, T., Cachau, R. & Joachimiak, A., Structural information content at high resolution: MAD vs. Native. (2003) *Methods in Enzymology*, accepted.)

1.03: High Resolution Structures

In recent years, the number of structures of biological macromolecules solved at sub-Angstrom resolutions has increased substantially, due to a series of methodological developments ranging from crystallization and data collection to better refinement algorithms. The purpose of this session was to review these developments and to show that the resulting structures can dramatically improve our level of knowledge about biological macromolecules in operation.

The program was thus divided in two parts: the first part, focused on methods, was led by **Andrzej Joachimiak** who opened with a very complete report of the current situation in subatomic resolution crystallography, explaining the methodological developments necessary at each stage. He showed the role played by high-brilliance synchrotron sources in these developments, and showed a variety of examples, including some from the 19 ID beamline at SBC, APS, which has played a leading role in collecting subatomic resolution diffraction data.

George Sheldrick described how density modification techniques could dramatically improve the quality of an experimental (MAD or SAD) map at subatomic resolution. He showed results on aldose reductase and thaumatin. The most striking result was the increase in the correlation of a thaumatin SAD map (phased with 2 sulfurs) with the correct one from 0.197 to 0.973. While he remains cautious about the validation of these methods, they clearly show great potential.

Bob Blessing described high resolution studies of hexameric complexes of zinc and insulin, focusing in particular on the allosteric transformations T_6 <--> T_3R_3 <--> R_6. These transformations control the rates of microcrystal dissolution and hexamer association important for the pharmacokinetics of insulin therapy. The high resolution structures of the T_6 (1.0 Å) and T_3R_3 (1.2 Å) conformations were the basis of a charge density study, which led to the electrostatic potential in the central core of the hexamers. The hydration structures around the hexamer centers appear to be implicated in triggering the T-> R transformation.

In the second part, focused on results and applications, **Nicholas Silvaggi** showed the details of the interactions of novel inhibitors of DD-peptidases with the R61 enzyme. Since these new inhibitors interact with the enzyme in unusual and unexpected ways, the high resolution (1.1 Å) was instrumental in validating these interactions. Two other talks also clearly emphasized the importance of high resolution in validation of interactions: **Ossama El-Kabbani** described the interactions of cyclic imide inhibitors Fidarestat and Minalrestat with aldose reductase (at 0.9 and 1.1 Å). The protonation state of both the inhibitors and the enzyme is crucial for the binding mechanism. **Yunfeng Tie** described the high resolution (1.6 to 1.1 Å) structures of complexes of inhibitors with HIV-protease mutants. These showed both the molecular basis of the tight inhibitor interactions and the structural changes associated with resistant mutations.

Chung Jung Chen showed an exceptionally accurate electron density, determined at 0.68 Å, for rubredoxin from *Desulfovibrio gigas*. In particular, the map in the region of the Fe-4S cluster showed the possibility of a second conformation, which might be important for biological function.

Several posters were also associated with this session. We can note the one by **M. Vamvouka** and **A. Mesekar**, in which analysis of mutants at 1.4 Å showed a proton shuttle for extradiol catalysis, and the one by **S. Ginell** et al, which reported high resolution structures (0.9 Å) of aldose reductase at 15 K and noted a clear diminution of the B-factors in the ordered zones.

In summary, it is clear that due to hardware and software developments atomic and subatomic resolution structures are becoming more common. The extra detail they provide can be crucial to the identification of function or inhibitor binding, so they serve to improve the power and scope of x-ray crystallography.

Alberto Podjarny

1.04: New Structures

Ten oral presentations were chosen out of over thirty submitted abstracts for the New Structures Session. The selected talks covered a broad range of biological systems, including receptors, transferases, polymerases, membrane proteins, and amyloid-like fibrils.

Gabby Rudenko presented the recently published structure of the low-density lipoprotein receptor (LDL-R; *Science* (2002) **298**:2353-8). Soaking sodium 12-tungstophosphate in the crystals serendipitously improved their diffraction quality and paved the way for a MAD structure determination. The completion of this project required growing 400 L of insect cells, engineering several point mutants, and collecting data on hundreds of crystals. But the resulting structure was well worth the wait, as it provided a possible mechanism for lipoprotein release in the endosome: At endosomal pH the ligand binding domain of LDL-R forms an arc over the rest of the protein. In this structure, two modules of the ligand binding domain associate to the beta-propeller domain via their calcium binding loops, thereby preventing lipoprotein binding.

1.04: New Structures, continued

Carnitine acetyl transferases play a crucial role in the transport of fatty acids and their dysregulation can lead to serious diseases in humans. The structure of carnitine transferase presented by **Gerwald Jogl** was solved to 1.8 Å resolution by the selenomethionyl single-wavelength anomalous diffraction (SAD) method (*Cell* (2003) **112**:113-122). The enzyme is made of two domains, which surprisingly share very similar polypeptide backbone folds. A three-dimensional query using the Dali server revealed that the domains share unexpected structure conservation with the chloramphenicol acetyl transferase.

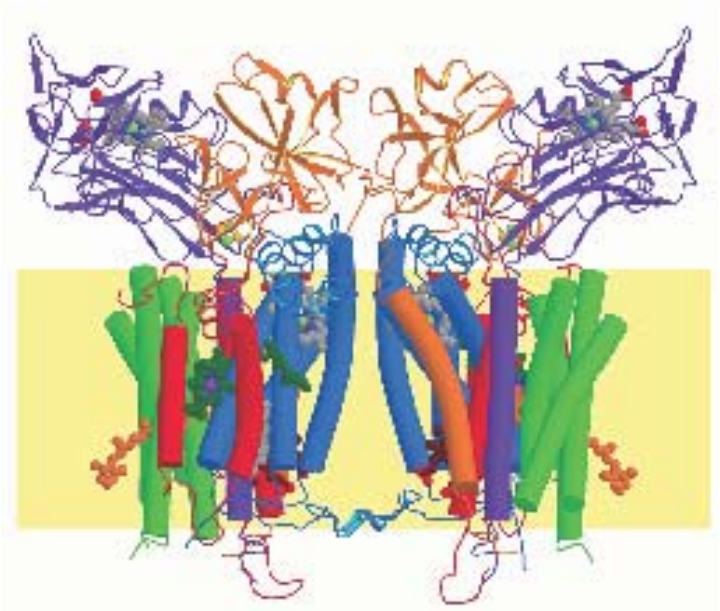
In the next talk **Maria Bewley** reported the structure of another acetyl transferase, the spermine/spermidine acetyl transferase (SSAT). SSAT is known to regulate polyamine levels in human cells, and deficiencies in this regulation are associated with human diseases such as Alzheimer's. The homodimeric structure, which was solved by selenomethionyl MAD, revealed that one subunit in the dimer was acetylated on a single lysine. A combination of biochemical and structural data led the authors to suggest that auto-acetylation is part of a novel regulatory mechanism of the ubiquitin-dependent degradation of SSAT.

Vivien Yee graciously agreed to step in for **Rui-Ming Xu** who had a last minute obligation and could not be at the meeting. Vivien presented the very first structure of a 2'-nucleotidyl transferase, 2'-5'-oligoadenylate synthetase (OAS), which unexpectedly turned out to be structurally very similar to poly(A) polymerase, a 3'-nucleotidyl transferase. Interestingly, the protein had to be treated with iodoacetamide in order to obtain diffraction quality crystals.

David Lodowski opened the second half of the session with the structure of the G-protein coupled receptor (GPCR) kinase GRK-2 in complex with the heterotrimeric G-protein subunits $\beta_1\gamma_2$ (*Science (2003)* **300**:1256-62). This critical kinase complexes to both GPCR's and to G-proteins, and the structure reveals how the GRK-2 pleckstrin-homology (PH) domain orients the kinase domain for action on a GPCR. David was the recipient of an Etter Student Lecturer Award from the ACA for this presentation *(see p. 13)*.

Brent Hamaoka then presented the 1.5 Å resolution structure of Her-1, a critical developmental module for male sex differentiation in *C. elegans*. Brent's structure revealed that mutations known to impact Her-1 function mapped to the interface between the two domains of the protein. In addition, it was reported that this structure was determined using Se-Met-substituted protein generated in Chinese Hamster Ovary (CHO) cells.

The structural examination of multisubunit RNA polymerases has greatly advanced our understanding of transcription initiation and elongation. **Katsuhiko Murakami** presented the next structures in this line of fine work – that of the bacterial holoenzyme (σ plus the $\alpha_2\beta\beta'\omega$ core) from *T. aquaticus* both alone, at 4 Å resolution, and in complex with an open promoter region at 6.5 Å resolution (*Science* (2002) **296**:1285-90). These structures reveal the placement of the elongated σ subunit, as well as the binding site of the fork-junction DNA promoter.



From Genji Kurisu: the sixteen-subunit dimeric complex from the thermophilic cyanobacterium, M. laminosus, is shown embedded in the membrane bilayer (yellow). The 26 trans-membrane helices are shown as cylinders, and other protein regions in ribbon form. Subunits are colored individually: cytochrome b_6 (blue), cytochrome f (purple), Rieske iron-sulfur protein (orange), subunit IV (red) and small subunits (green). Seven cofactors per monomer are shown in the figure: four hemes (gray and brown), one iron-sulfur cluster (green-yellow), one chlorophyll a (green) and one β-carotene (orange) per monomer. The structure was solved at Purdue University by Kurisu, Zhang, Smith & Cramer.

Proteins translocated into the endoplasmic reticulum (ER) of eukaryotic cells are translated on ribosomes recruited to the ER membrane by the signal recognition particle (SRP) and its membrane-associated receptor (SR). **Tom Schwartz** presented the 1.7 Å resolution structure of the dimeric SR complex of G proteins SRα and SRβ bound to GTP (*Cell* (2003)**112**:793-803). The structure, combined with biophysical data, indicated that SRβ may be a regulatory switch controlling receptor dimerization.

John Hart then presented structures of pathogenic mutant forms of human superoxide dismutase linked to the development of familial amyotrophic lateral sclerosis (ALS). John's structures revealed amyloid-like fibril formations in molecular detail that mimic fibrils observed in ALS motor neurons (*Nat. Struc. Biol.* (2003) **10**:461-7). The mutations in superoxide dismutase that promote the fibril formation generated novel β-stranded interactions critical to polymer stabilization.

Genji Kurisu wrapped up the session with the report on the cytochrome b_6f complex. This large and critical membrane protein is a component of the photosynthetic electron transfer chain and has been examined for decades. Nonetheless, this first crystal structure, at 3.0Å, revealed an unexpected additional heme that had eluded biochemical detection.

Sylvie Doublié and Matt Redinbo

1.05 Protein Structure, Function and Dynamics

Motion is fundamental to protein function. This session extended the crystallographic view of protein conformational dynamics far beyond atomic vibrational factors. Here we have begun to capture proteins' dynamic states (their rough energy landscapes) and link these to protein function.

George Phillips began the session with a refinement method that treated overall protein motion by the Gaussian network model but with added lattice contacts. He compared this with a rigid-body librational model of vibrational motion. Correlation of the B values depends on the molecular shape with improved agreement for non-spherical proteins with this model.

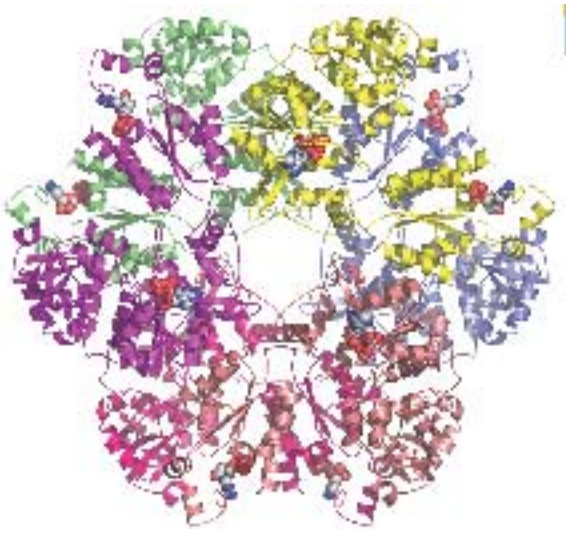
The allosteric protein systems in the next two talks showed that small interactions can trigger correlated conformational changes. **Bog Stec** found that, in crystals of a mutant of allosteric FPBase, 4 distinct states of the protein could be trapped, 2 ~ R and 2 ~ the S state. These crystals effectively sampled the rough energy landscape of the protein and revealed new information about its allostery. **Andy Fisher** showed movies of the R/T transition of allosteric ATP sulfurase. The T state complex binds two molecules of product APS in different ways. Loss of a salt bridge between the catalytic and allosteric (regulatory) domains of adjacent proteins in a trimer results in an R to T state transition. Interestingly, the C-terminal allosteric domain is homolgous to APS kinase that catalyzes the next step in the synthesis of the sulfate donor PAPS.

Lukasz Lebioda found crystals of neuron enolase homodimers adopted asymmetric loop conformations (open, closed and half-closed) and described how this can aid in inhibitor design. **Ewa Ciszak** showed dramatic rearrangments in pyruvate dehydrogenase, where coordinated movements of heterodimers provide an explanation for the flip-flop mechanism of this protein. **Catherine Regni** demonstrated how the same protein phosphomannomutase / phosphoglucomutase can catalyze both 1- and 6-phosophoryl transfer in glucose or mannose by changing a flexible active site. **Ann McDermott** educated crystallographers on the value of using multiple biophysical approaches to really understand time-dependent processes. **Martha Teeter** finished the session by showing how coupled crystal alternate side chain conformations in myoglobin at a 1 Å resolution can provide pathways for ligand migration. Migration of cavities due to alternating discrete disorder around the heme provides a mechanism for the unexplained migration of CO from one side of the heme to the other.

Martha Teeter

From left, in front: George Phillips, Ewa Ciszak, Martha Teeter, Bog Stec, Cathy Regni; in back: Lukasz Lebioda, Ann McDermott, Andy Fisher.

Below, from Andy Fisher: Structure of hexameric ATP sulfurylase from the fungus Penicillium chrysogenum. The enzyme catalyzes the adenylyl transfer of ATP to sulfate as part of sulfur assimilation pathway and is allosterically inhibited by PAPS (the product of the second reaction). The structure shown contains APS bound both to the active site and the allosteric effector binding site and represents the active R-state of the enzyme.



Posters: Proteins with Structure and Function Emphasis

Karen McLuskey presented P042 on the *E. coli* enzyme MobB, which along with MobA is involved in the attachment of nucleotide to the molybdenum cofactor. The 1.9Å structure revealed that MobB is made up of 2 domains and forms a dimer. A very interesting feature of this dimer is that the minor domain (two β–strands and a α-helix) from each subunit inserts between the major and minor domains of the other subunit in a "domain-swap" interaction creating a stable molecule with a continuous 16-stranded β-sheet. MobB is reported to posess GTPase activity but unfortunately, no GDP was seen in the electron density map. Instead a sulfate ion was present binding in the Walker-A motif. The authors also propose an interesting model of a complex between the MobB dimer and MobA dimer with bound GTP that fits neatly into a pocket formed at the protein-protein interface.

Svetlana Pakhomova (LSU) presented P059 on the flexibility of fosfomycin resistance protein FosX. This metalloenzyme represents the second fosfomycin resistance protein determined in the lab. An interesting attribute of this structure is that the authors solved the structure from three different space groups grown at four different pHs (one space group at 2 pHs). Comparison of the structures revealed significant conformational differences in loops near the active site that may modulate activity. These structures will lead to a better understanding of how some bacteria gain resistance to the antibiotic fosfomycin.

Structure-Function Posters, con't

Kiira Ratia from U. Illinois-Chicago (P086), using directed evolution to increase activity of a novel phosphotriesterase. Phosphotriesterases are a class of enzymes that are capable of hydrolyzing potent neurotoxins such as Sarin, Soman, and VX. Especially because of recent terrorist activities, there is much interest in developing agents that detect and destroy potential chemical warfare agents. These authors used error-prone PCR to identify mutations that increased activity in hydrolyzing potential chemical agents. They were able to identify mutations that increased catalysis by 50-fold over paraoxon and coumaphos. Surprisingly, most of the mutations mapped to the dimer interface of the enzyme, and not near the active site, which the authors suggest may open up the active site pocket allowing for faster product release.

Cory Momany, U. Georgia, presented P090 on effector binding domain of BenM, a transcript regulator involved in benzoate metabolism. The dimeric structure consists of two α/β subdomains in each monomer. The two binding pockets, one of which contains a sulfate ion, are separated by 20Å. We anxiously await the structures of the domains with bound effectors to better understand atomic detail of transcriptional regulation (work in progress).

Wolfram Tempel from B-C Wang's group at Georgia presented P094 on the mammalian Class I Golgi α1,2-mannosidases, which are critical enzymes in the maturation of N-linked oligosaccharides. This project stemmed from their high-throughput crystal structure determination project. They solved the structure from sulfur anomalous scattering on an in-house rotating anode. The structure (with $(\alpha\alpha)_7$ barrel topology) is similar to other Class I mannosidases from the ER. An interesting finding in this structure is that the active site is occupied with the oligosaccharide from a N-linked $Man_5GlcNAc_2$ of a symmetry related molecule. However, the binding conformation of the oligosaccharide differs from that observed in previous ER mannosidase structures.

Maria Miller, U. California, Berkekey, and coworkers (P49) further characterized DNA recognition by C\EBP transcription factors. The interplay of dimerization requirements with the requirements for fitting the electrostatic features of alpha-helices resulted in a fork-like structure that interacts with DNA, generating a highly specific system.

Young Do Kwon, NCI, and coworkers, (P0121) reported on an imaginative structural approach towards elucidation of the role of pro-peptide in proteasome self-assembly.

Andy Fisher and Lukasz Lebioda

In back, from left, Onkar Singh, Igor Jurisica, Andrzej Joachimiak, Zygmunt Derewenda, Peter Kuhn, Alex Burgin, David Waugh, Dawei Lin.

1.07: High-Throughput Crystallography

The session featured eight speakers whose presentations covered the range of procedures in high-throughput protein crystal structure determination, from gene design to crystallographic computations. The speakers presented new methods and techniques to increase the output, not just the throughput, at each step.

Alex Burgin from deCODE genetics presented new methods in whole gene synthesis. Ample protein production by recombinant methods is usually the first step in protein structure determination. Often, protein production is stalled due to poor expression. One of the factors in poor expression is non-optimized codon usage for the given expression system. By designing genes based solely on the final amino acid sequence of the target protein, silent mutations at the gene level can be introduced with optimized codon usage for the particular expression system. Furthermore, restriction sites and purification tags can be easily introduced into the gene. Novel software has been developed to design genes for whole gene synthesis. This software designs genes and the oligonucleotides to make these genes. In addition to codon usage, the software designs genes according to other criteria, such as minimizing the variance in melting temperature and secondary structure in the oligos.

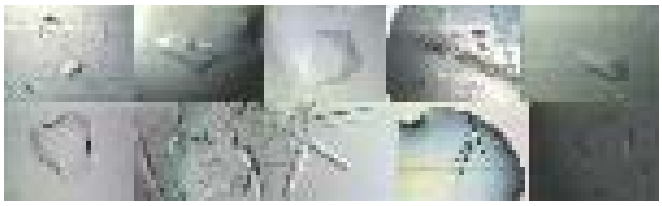
David Waugh, NCI, described a generic strategy for protein production in *E. coli* that utilizes a dual, N-terminal His6-MBP tag. The MBP moiety improves the yield and enhances the solubility of the passenger protein while the His-tag facilitates its purification. The soluble fusion protein (His6-MBP-passenger) is purified by immobilized metal affinity chromatography (IMAC) on Ni-NTA resin and then cleaved *in vitro* with His6-tagged tobacco etch virus protease (His6-TEV protease) to separate the His6-MBP from the passenger protein. In the final step, the unwanted byproducts of the digest, as well as any impurities that eluted from the Ni-NTA resin along with the fusion protein in the first IMAC step, are absorbed by a second round of IMAC, leaving nothing but the pure passenger protein in the flow-through fraction. This simple generic protocol should be readily amenable to automation for high-throughput applications.

Onkar Singh from GlaxoSmithKline (GSK) presented a crystallization setup and management system developed by GSK and Data Centric Automation (DCA). One of the primary factors motivating the development of a crystallization platform is that modeling is not enough. Experimentally determined protein structures are required for drug design and development. In-house development of an automated crystallization platform would be too resource-intensive. Commercially available systems suffered from limited range of experiments and data capture. The Rhombix OPUS automated crystallization system developed by GSK and DCA combines several commercial instruments on a unique single platform. All steps in

1.07: High-Throughput Crystallography, con't

the crystallization process, from solution making to plate sealing, are automated. The system is capable of setting up sub-microliter volume crystallization drops, and uses 10-fold less protein than traditional manual methods. The hardware can store more than 500 SBS format crystallization plates, and the software can handle more than 50 screening and optimization projects at one time.

Zygmunt Derewenda, U.Virginia, presented techniques in the surface mutagenesis of proteins to enhance the likelihood of useful protein crystallization. He remarked that the most important parameter in the crystallization experiment is the protein itself. A large entropic cost in protein crystallization is the stabilization of large charged side chains, particularly lysine and glutamic acid, which are correspondingly underrepresented in crystal contacts. About 94% of lysines and 88% of glutamic acids are found on the surface of proteins. Mutating these large residues to alanine reduces the entropic costs of crystallization, and can result in more useful crystallization. Replacement of single Glu or Lys residues tended to change the rapidity of crystal formation, while double- and triple-mutants resulted in new crystal forms for the proteins. Results were presented for several proteins, including the LcrV antigen from *Yersinina pestis* whose native form could not be crystallized. Surface mutagenesis on this and other proteins led to crystals of x-ray diffraction quality.



From Zygmunt Derewenda: The K2A series of crystals. Single and multiple Lys -> Ala and Glu -> Ala mutations critically alter RhoGDI's ability to crystallize, (Longenecker et al (2001) Acta Cryst. D57: 679-88 and Mateja et al (2002) Acta Cryst. D58: 1983-91.

Igor Jurisica (Ontario Cancer Institute) presented automated image analysis of 1536-well microbatch crystallization plates, developed in collaboration with the Hauptman-Woodward Medical Research Institute. The ultimate objective of this study is to determine a signature or fingerprint for a protein. Proteins that have similar signatures react similarly under a wide range of crystallizing conditions, and thus should crystallize under similar conditions. In turn, determining such protein fingerprints may lead to quicker crystallization of a target protein. The steps in the automated classification of the crystallization images were location of the crystallization drop, droplet segmentation, and 23-element feature extraction. Using a human expert's observations as the standard, the automated image analysis was 89% accurate.

Peter Kuhn (Scripps Research Institute) presented the data centric approach of the Joint Center for Structural Genomics (JCSG) to the entire protein structure determination process, from protein expression to crystallographic computations. It was noted that, by the process flow diagram developed, there were 69 points of potential human error in the structure determination of a single target protein. A web-based database application has been developed to track 300 individual parameters in the structure determination process. Protein expression, crystallization imaging, and crystal harvesting were noted as particular bottlenecks in the process. The Blu-Ice software is the synchrotron diffraction data collection interface. A cryo-cassette has been developed which holds 96 frozen crystals. Increased diffraction screening of crystals for a given target protein enhanced the likelihood of obtaining a well-diffracting crystal for structure determination. In the structural genomics study of *Thermotoga maritima*, 2,411 crystals from 179 different protein targets were screened, and 65 different protein structures have been determined.

Dawei Lin (U.Georgia), presented a pipeline system for automating crystallographic computations based on work flow technology. The objective of the pipeline system is to relieve the human researcher of the tedium of trial-and-error adjustment of computational parameters, and allow the human researcher time for other tasks. The system is web-based and database driven. It was based on bioPerl-pipeline, an open source work flow system. The system is mainly written in Perl. Molecular replacement computations with AMORE, phasing of anomalous signal with SOLVE/RESOLVE, and electron density map tracing with ARP/wARP have been implemented in the system. The pipeline was used to determine several structures that had not been solved by months of manual crystallographic computations. The structure of a novel protein from a structural genomics project was solved in 4.5 hours using the pipeline, after processing the diffraction data.

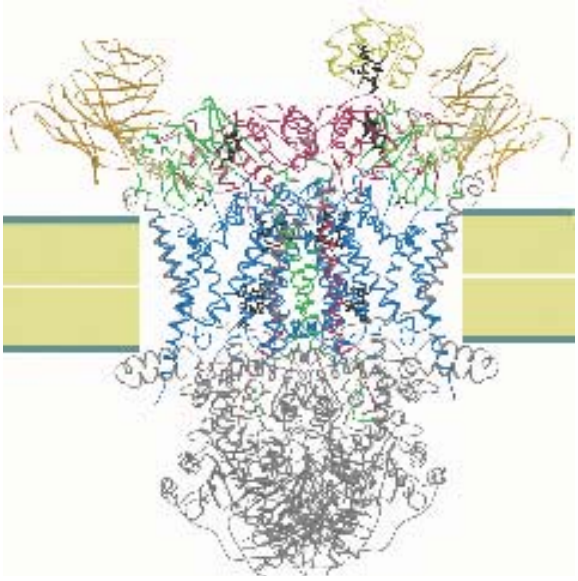
Andrzej Joachimiak (Argonne) closed out the session with a review of the current state of progress of the Midwest Center for Structural Genomics (MCSG). It was noted that of the more than 800,000 genes from 120 completed microbial genomes, 13,558 gene families have no sequence homology with structures in the PDB. Expressed proteins are purified by AKTA Explorer 3D chromatography workstations using semi-automatic protocols. Proteins are assayed by several methods, including dynamic light scattering. Crystallization plates are set up by a combination of the Cartesian and Hydra robots. PEG/salt vs. pH grid screens have been highly effective for protein crystallization. His-tag cleaved proteins have shown a slightly higher rate of crystallization. Protein structures have been determined mostly by Se-Met MAD and SAD. MAD has been used most often, but for one SAD case, 1 Se-Met was used to phase 297 residues. Usually, more than 10 crystals for a given target protein are screened for diffraction before collecting the full data set. Of 1,457 targets cloned, 237 proteins have been crystallized. Thus far eighty-one different protein structures have been determined at MCSG, of which 13 are novel folds.

Hidong Kim

"Amorphous Phase" from Charlie Carter's talk on Prickly Mountain Project. ***see p. 28.***

1.08: Membrane Protein Structures

In introducing the Membrane Proteins session, **Hans Deisenhofer** noted that twenty one years earlier, almost to the day, Hartmut Michel had presented at a meeting in Erice the diffraction pattern of the first membrane protein to be solved crystallographically, the photosynthetic reaction center from *Rhodopseudomonas viridis*. Although progress through many of these intervening years has been frustratingly slow, the recent explosion of membrane protein structures has created a sense of excitement in the field that was beautifully captured by the speakers of this session. **Carola Hunte** provided a clear overview of the problems, and their current solutions, inherent in the study of membrane protein structures. She stressed the challenges of low natural abundance, the need to provide a suitable mimic for the membrane environment, and approaches to stabilizing lattice contacts through the use of antibodies to improve crystal quality. These issues were exemplified by her structural studies on cytochrome bc_1 illustrating the pathways of proton and electron transfer in this respiratory complex.



From Carola Hunte: Structure of the electron-transfer complex between cytochrome *c* (yellow) and the cytochrome *bc*1 complex (QCR) with bound antibody Fv fragments (orange). The specific interaction between the two redox partners of the respiratory chain allows fast electron transfer and reversible docking of the mobile electron carrier cytochrome *c*. The latter binds only to one of two possible binding sites of the homodimeric QCR. The catalytic subunits cytochrome *b*, cytochrome *c*1 and Rieske protein are coloured in blue, red, and green, respectively. The relative position of the inner mitochondrial membrane is indicated. (Lange, C., Hunte, C. (2002). Crystal structure of the yeast cytochrome *bc*1 complex with its bound substrate cytochrome *c*. *Proc. Natl. Acad. Sci.* USA 99, 2800-2805.)

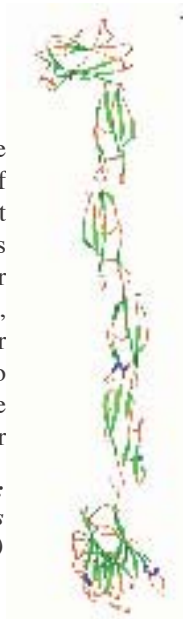
A highlight of this session was the presentation by **Jeff Abramson** of the structure of lactose permease that couples lactose transport to a chemiosmotic gradient. The substrate binding site is positioned at the interface of this bilobal transporter, and the flow of protons through the system drives conformational rearrangements that alternatively open this site to opposite sides of the membrane. **Geoffrey Chang** presented his structural analysis of a representative of a family of active transporters that couple ATP-hydrolysis to the translocation of ligands, such as lipids and drugs, from one side of the membrane to the other through a scissors-type mechanism that controls access to the ligand binding site. Transporters for ferric citrate and vitamin B_{12} across the outer bacterial membrane were described by **Wyatt Yue** and **Michael Wiener**, respectively. These homologous transporters are organized around a 22 stranded antiparallel β-barrel with a plug in the middle, raising the challenging question of how ligands get around, or through, the plug. The session closed with **Michael Rossmann**'s elegant presentation of viral membrane proteins found in flaviviruses, using a combination of cryoelectron microscopy and x-ray crystallography to study conformational changes in the viral lifecycle.

The progress made in overcoming experimental obstacles to sample preparation, the availability of high-intensity synchrotron sources and other crystallographic resources for structure determination, and the number of outstanding structural targets portend many exciting developments in the field of membrane protein structure over the next twenty one years and beyond.

Hans Deisenhofer and Doug Rees

Posters: Interesting Macromolecular Structures

The poster hall in Covington bustled with a rich mix of puzzles, new methods and unexpected structures. The first known proline dehydrogenase, which also binds DNA, (PutA flavoprotein, P29, **John Tanner**), was one of many interesting new structures presented. Another poster, (P83, **Alexey Dementiev)**, described a serpin mutant α_1-PI$_{Pittsburgh}$ that causes a fatal bleeding disorder, in complex with trypsin. One of the more surprising structures was a large (79 kDa) new *B.t.* insect toxin that has 6 domains arranged in a long row, (P209, **Tim Rydel**). Another protein complex with both structural interest and health relevance was the ActRIIB:Activin A complex, (P34, **Thomas Thompson**). This structure adds new depth to the busy family that includes transforming growth factor beta (TGF-β), activins, and their receptors. The list of notable posters could go on and on; I'll limit myself to mentioning three more. Under "mysteries of metabolism," P 223, **Angela Toms**, contributed to the still incomplete science of thiamine biosynthesis by describing the structure of TenI, which is one of several proteins needed for thiamine biosythesis whose exact functions are still unknown. A SlyA transcription factor from an *Enterococcus* pathogen, with provocative phylogenic relations to other expression-modulating factors, was also colorfully described, (P10, **R-y Wu**) and finally, yet another carefully composed poster illuminated and analyzed a novel class of three-heme cytochrome domains (P99, **Raj Pokkuluri**).



From Tim Rydel: Cry22-class Bacillus thuringiensis (B.t.) toxin structure.

Travis Gallagher

Socializing on Riverboats, the Bruker/Nonius and Ohio Riverboat Dinner Cruises.
Top, from left: Andy Howard and Peter Lee; Ann Wolff, Sharon Davis, Ray Davis and Khalil Abboud.
Upper middle: Grazyna and Andrzej Joachimiak and Kottayil Varughese; Magician with (seated) Jim Viccaro and Philip Coppens.
Next: Vickie and Rick Staples; Marilyn Olmstead; Fred Hollander.
Bottom, from left: Alex Yokochi, Jim Britten, Hamilton and Helena Napolitano; Joyce and Jim Ibers.

Protein Posters: Emphasis on Enzymes

The macromolecular crystallography poster sessions presented quite a diverse collection of crystal structures, the majority of which were enzymes. The investigators focused on the insight provided by these structures into the molecular basis of the catalytic mechanisms.

In P057 **Robert McKenna** (UFL) and co-workers presented the structure of carnitine acetyltransferase. This unique molecule contains two equally sized α/β domains that are arranged in such a way that they form a narrow active site tunnel, a possible universal trait for other carnitine acetyltransferases. There were several different synthetases presented at the meeting (e.g. threonine synthase, P064, inositol-1-phosphate synthase P118, pantothenate synthetase, P077, argininosuccinate synthetase, P084, and phosphopantothenoylcysteine synthase, P219). The structure of pantothenate synthetase from *M. tuberculosis* was presented by **Shuishu Wang**, UCLA (P077). The pantothenate synthesis is essential for virulence of *M. tuberculosis* and might serve as a potential drug target against tuberculosis. The crystal structure of the complex with reaction intermediate, pantoyl adenylate suggests that its analogs may serve as good inhibitors. The structure of human phosphopanthothenocysteine (PPC) synthase, P219, presented by **Narayanan Manoj**, Cornell, revealed similarities to several NAD-dependent enzymes and a ribokinase fold. Modeling and structural homology studies helped in finding the positions of the binding sites for ATP, phosphopantothenate and cysteine. Based on these studies the authors postulated a ping pong mechanism for formation of PPC. Finally, a structure of C-terminal domain D3 of bioluminescent luciferase (LCF) from scintillons of marine dinoflagellates that emit flashes of light regulated by circadian clock, was presented in P051 by **L. Wayne Schultz**, UW-Madison. Dinoflagellates are algae responsible for much of ocean luminescence.

Non-enzyme structures were less popular this year. The crystal structures of N-terminal non-catalytic DCX domains of doublecortin-like kinase (DCLK) and doublecortin (DCX) were presented in P097 by **Myung Hee Kim**, UVA. The crystallization of N-DCX is yet another example of crystallization by a powerful technique of surface entropy reduction. The DCLK and DCX proteins are associated with severe malformation of human cerebral cortex. DCX was reported to function as microtubule-associated protein (MAP). The functional studies of these proteins are being based on the distinct structural similarities to the Ras-binding domain of the ubiquitin superfamily. **John Gately Luz**, Scripps (P231) showed the crystal structure of XOL-1, a primary sex determinant in *C.elegans*. Unexpectedly, despite minimal sequence homology the protein structure identified XOL-1 as a member of GHMP kinase family. This fact may help in understanding of the protein's role as a developmental regulator.

The emphasis on enzymes at the ACA poster session is probably a result of an exodus of crystallographers interested in cell regulation and other aspects of biology to other meetings. As crystallography matures and transforms into an analytical tool in the hands of biologists, this trend is likely to continue.

Zygmunt Derewenda

Fiber-SIG sessions

This year Fiber-SIG organized one half day session **2.01:** ***Characterization of Biological and Medical Fibers*** and co-organized two sessions with SAS-SIG **8.03:*Advancements in Instrumentation for the Scattering and Diffraction Sciences*** and **8.01:** ***Probing the Frontier of Soft Condensed Matter Science with Small Angle Scattering.***

The Fiber SIG session was sponsored this year by FiberNet, which is a NSF Funded -"Research Coordination Network" for Fiber Diffraction from Biological Polymers and Assemblies. As part of the session, **Gerald Stubbs** gave a talk describing this new initiative which aims to coordinate fiber diffraction activities in the USA and cooperate with other groups, particularly CCP13 in Britain and BioCAT at APS. Its main actvity will be to develop biological fiber diffraction methods. and to sponsor retreats and workshops at the BioCAT facility at the Advanced Photon Source, State Park retreats, and fiber diffraction sessions at meetings of the ACA.

Fiber SIG Business Meeting:

Paul Butler gave a presentation concerning ideas for reorganizing the SIGs and their activities to improve coordination between the SIGs and to make the ACA meeting more valuable. His main proposal was to lengthen terms of officers to improve institutional memory and to develop a structure to improve coordination between the SIGs. The SIG membership present agreed that these were worthwhile goals. In light of this discussion, a proposal to change the SIG constitution to change the numbers of officers and terms of office was tabled until this process was further along.

A nominating committee was formed of Gerald Stubbs and Joseph Orgel. The current chair, Tom Irving, was charged with choosing a third person for the committee from the SIG membership. The nominating committee is charged with selecting candidates for upcoming ACA elections for SIG Chair and Secretary-Treasurer.

It is anticipated that Fiber SIG, according to recent practice, will sponsor a technique-specific session once every two years alternating between sessions with a biological focus, and those with a non-biological focus. The chair -elect will be responsible for organizing a session in 2005. The SIG will continue to co-organize with other SIGs joint sessions of mutual interest. For the 2004 meeting Fiber-SIG will co-organize a session with the Synchrotron Radiation SIG. *Tom Irving*

Photo by Ross Doyle: Jellyfish at Newport Aquarium

Sessions Organized by the General Interest Group (GIG)

3.01: This first GIG session was devoted to a mixture of topics, in keeping with the aim of the group. Attendance ebbed and waned, averaging about 30, with peaks for I.D. Brown's and Herb Hauptman's presentations (more than 70). It was particularly pleasing to see both old timers and new folks. Apparently there still is general interest amongst the meeting's attendees.

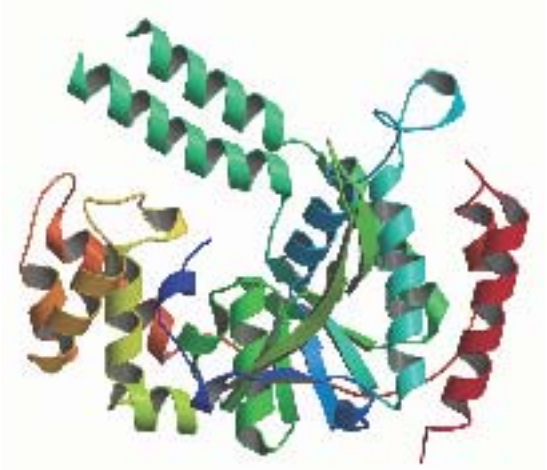
The session started with **Mikhail Antipin** presenting work related to his development of organic chromophores for wavelength conversion (SHG and beyond) which gave a good overview, as well as some new results in the area, with a brief discussion of the effect of polymorphism in materials' performance. **Mladen Barbic** described *Magnetic Resonance Diffraction*, a proposed imaging technique which, by taking advantage of very high magnetic field gradients generated by micro beads of magnetic materials, should be able to probe individual planes of unit cells. He covered the history, theory and some simulation results of this method, which could lead to a novel tool to investigate crystalline materials. **Michael Ruf** described the philosophy and some results of a new de-twinning routine; part of Bruker's software package which includes some brute force autoindexing methods for recalcitrant crystals. **I. David Brown** described a simple electrostatic model that adequately describes relationships in the bond-valence/bond-length/bond-compressibility space for ionic compounds. **Qun Shen** presented a technique to accurately measure three beam diffraction patterns using a new 5 circle + area detector diffractometer, as well as a modified dynamical/kinematic approach (using only 2 term effects) to fit the measured interference intensities. **Jeffrey Roach** expanded his previous year's presentation on the use of *local squaring functions* which describe the scattering function of a complete group of atoms. These can be used to improve the refinement of macromolecular structures for which only low resolution data is available. Finally, **Herbert Hauptman** shared his latest experiences with the *Phase Problem in Neutron Crystallography* and some misconceptions about its solution. Namely, he proposed that it is a major misconception that positivity is a requirement for structure solution by direct methods, and that comparisons between real x-ray data and simulated neutron data for several compounds using the Shake-and-Bake and Neutron Shake-and-Bake programs showed a much higher rate of correct solution determinations for the neutron data sets.

Alexandre Yokochi

3.02: This was an eclectic session with interesting topics that covered instrumental and practical aspects of crystallization, diffraction, and phasing, issues of color recognition and display, and theoretical calculations for heat transfer in protein crystals. It was so well attended that we moved to a larger room after the coffee break. **Boris Verman** described new x-ray optics, and showed that optimization for either flux or resolution requires different sets of optimized optics. **Randy Alkire** then described his analysis of the dependence of air scattering of x-rays on the distance between sample and beam stop at APS 19 ID, concluding with the suggestion that the beam stop be placed as close to the sample as practical, and that low resolution reflections be measured as a separate pass with the beam stop placed further away. **Zhi-Jie Liu** described the usefulness of an in-house Cr x-ray source in structure determination by sulfur phasing, extending on phasing methodology which was originated by Bi-Cheng Wang "in the last millennium". **Marc Allaire** presented his analysis of multi-chromatic beam diffraction geometry, and concluded with the very useful parameters of a minimal 1.5 mm spot separation, which would require a 0.1 km detector distance in order to discriminate between diffraction spots for Se inflexion and peak wavelength datasets. **Joseph Ng** then described how crystallization and measurement of all data required for structure determination can be carried by in-capillary counter-diffusion, minimizing the need for crystal manipulation. Hey Joe, how about adding in-capillary protein purification? **Herbert Bernstein** gave an entertaining and thought-provoking presentation on the variation in human recognition of colors, and provided suggestions on how to accommodate different types of color-deficiency and -blindness. **Michael Kazmierczak** finished the session off by describing detailed calculations of heat convection and conduction in cryo-cooled protein crystals upon x-ray exposure.

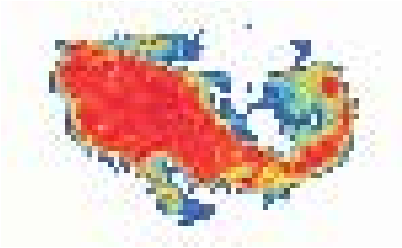
Vivian Yee

3.03: As usual for a general interest session, there was an interesting mix of topics. The first collection of talks included one from **Artem Evdokimov** (Proctor and Gamble) on the use of methionine aminopeptidase inhibitors as a possible source of future antibiotics. It was good to see some of the typically proprietary and secretive work carried out at a corporation. One of the surprising things from this talk was that, for this case, all of the candidate compounds designed by the super computer failed to bind to the active site. The human designed ones did a much better job. In the next talk, **Steve Tomanichek** needed to flex more than his biceps to solve the structure of the crenarchaeal aeropyrum flap endonuclease 1, which is a DNA repair enzyme. In the structure, there was a floppy disordered loop that Steve speculated might be important for DNA binding. As Sheldrick was giving a talk in an opposing session, we lost a large portion of the audience before Steve's talk.



From Steve Tomanicek: Structure of a DNA repair Flap Endonuclease-1 (FEN-1) enzyme from a crenarchaeal organism that functions at temperatures upwards of 70°C.

3.03, con't: **Pamela Hall** discussed structural work related to the transcarboxylase multienzyme complex. She had some amazing 3D animations of the complex at work including one that looked similar to the human embryo-farming robot from *The Matrix*. After the break, **Govinda Lakshamanan** discussed the structural results from parvoviruses and how certain areas of the virus are host dependent for this particular disease. **Unmesh Chinte** discussed the glycerol concentration required to vitrify samples with helium and nitrogen. He described a thermodynamic model of the cryostream indicating a 0.5 mm radius around the middle of the stream where cooling is consistent. This was verified by measurements made in the cold stream. Finally, **Jeff Lovelace** gave a talk on the use of a CCD surveillance camera to record topographs. His talk included a replay of a series of captures leading up to and including the first topograph highlighting the agony of defeat and the thrill of victory. The speakers all kept to their alloted time, which allowed for many questions and lively discussions. *Jeff Lovelace*



Comment by Gloria Borgstahl, session organizer:

This picture (shown by Jeff Lovelace) generated much nonscientific discussion at the General Interest III session. Some people thought it was an image of the future US after a flood as seen by some psychics; others thought it resembled a fish. Actually, it was a digital topograph from a cubic insulin crystal taken with a modified surveillance camera .

3.04: The session began with crystallographic point groups and ended with pointers to online tutorials on crystallography. Pertinent points raised in response to questions put to speakers **Larry Falvello** and **Peter Müller** addressed how each would integrate the subject matter into their teaching. There were interesting conversations at the close of the session and continuing afterward on how to create/improve online tutorials and ease access to the information. Though all was educational, the overall point of the session was not only education. The design and interface of the Reciprocal Net was featured; the tag-team of **John Bollinger** and **John Huffman** presented an online structural database, primarily for small molecules, that is distributed in architecture over several servers. A given laboratory has full control over just what information is made public. **Jonathan Schuermann** gave a to-the-point demonstration of how SAD phases flushed-out the correct MR solution from an initially intractable situation. Jonathan's talk left plenty of time for the presentation of a 2003 **Etter Student Lecturer Award** to **Jennifer Padilla.** Jennifer then educated us on how crystal contacts between macromolecules explain the observed occurrences of space group symmetries.

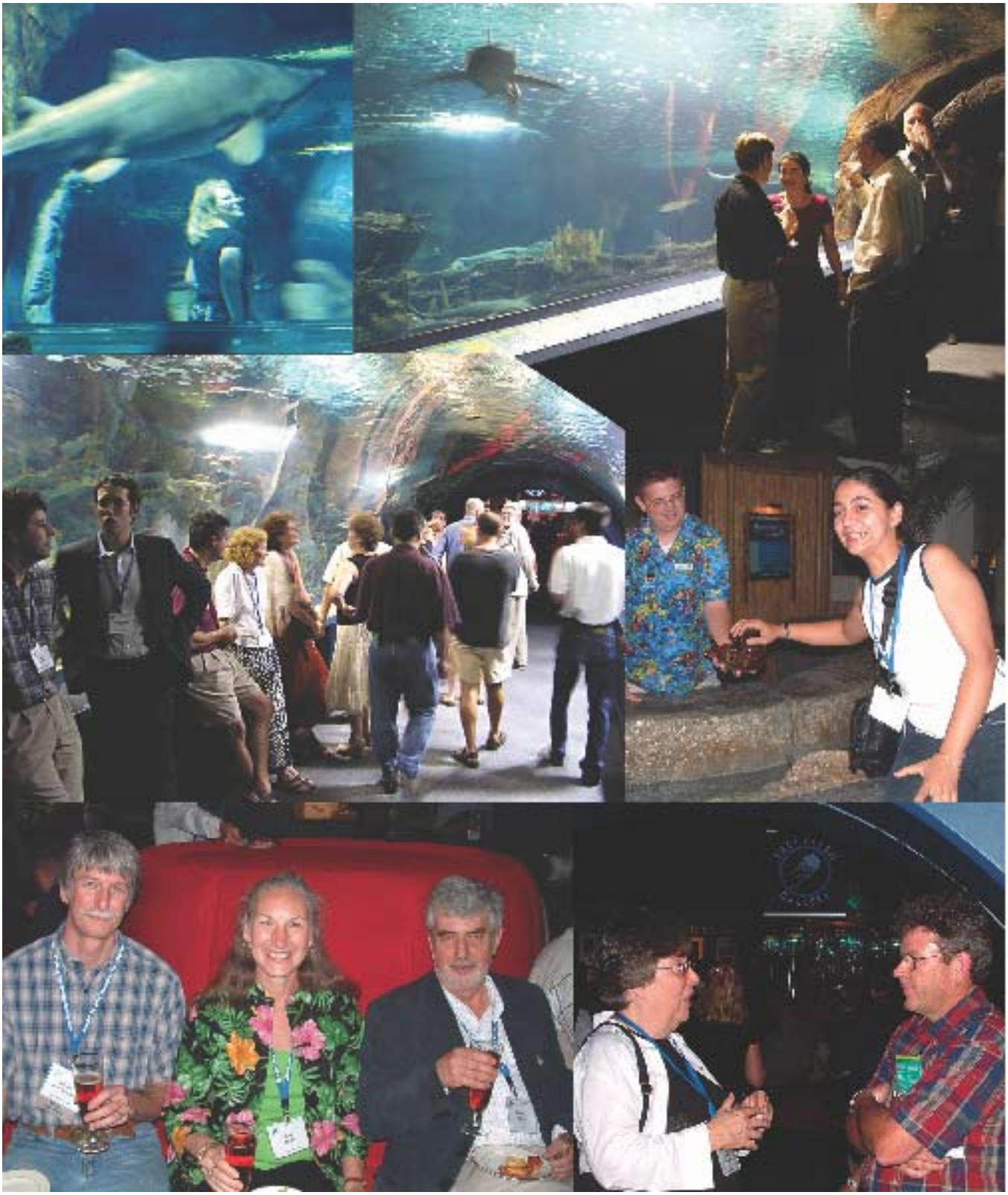
Jim Thompson

3.05: The 5th GIG session took us on a whirlwind tour through conformational changes in proteins to ligand binding, with a quick detour under the direction of **William Heller** into the use of SANS to probe the effect of phosphorylation on the formation of troponin complexes in solution. Although the crowd was a little rowdy (clearly looking forward to the end of meeting drinking session) the speakers coped well with the post coffee break heckling and told us about some great science. Conformational changes ranged from the breathing motions reported for the active site loop of TIM by **Ricardo Aparicio**, to the whopping 140° rotation **Andrew Gulick** told us about in acetylCoA synthetase which is required to control the two-step catalytic reaction. **Kunchithapadam Swaminathan** gave us insight into the way fungi cope with wounds by using HEX-1 and the Woronin body as a plug to stopper leaky cell junctions. **Lesa Beamer** presented a high resolution structure of the GDP-mannose dehydrogenase from *P. aeruginosa*, with an interesting domain swapped architecture that will hopefully provide a starting point for antibiotic design. **Eric Schreiter** showed how the structure of the Nickel dependent transcriptional repressor, NikR, from *E. coli* explained some its DNA binding properties. The final talk of the session by **Schoen Kruse** was, perhaps appropriately, on the LUSH protein. LUSH is the alcohol receptor of drosophila and Schoen explained how the structure has given insight into the binding of alcohols to proteins. *Arwen Pearson*

FromSchoenKruse:ribbondiagram of the LUSH-Butanol structure (at 1.25 Å). Butanol is represented as a space-filling model at the center of the protein (alkyl chain, cyan; hydroxyl group red). Described in: Kruse, S.W., Zhao, R., Smith, D.P., Jones, D.N.M., Structure of a specific alcohol-binding site defined by the odorant binding protein LUSH from *Drosophila melanogaster*. *Nat Struct Biol* 10:694-700 (2003).

General Interest Posters

The General Interest Posters contained an interesting mix of math, physics and materials science. **Randy Alkire**, Argonne, P129, presented the effect the distance of the beam-stop has on air scatter. The study indicated that the closer the beam stop is to the sample, the better, data quality decreases with increasing distance. If low resolution data are needed, collect one set with the beam-stop close and one with it far. **Malgorzata Rowicka**, U. Texas, P133, presented the use of 4-vector notation (instead of 3) as a means of simplifying complex terms, allowing vectors to be described and manipulated more easily, thus making life simpler for the software programmer, particularly for debugging software. And **Maureen Julian,** P135, gave an enthusiastic tour through the methods she uses to instruct undergraduate and graduates in Materials Science at Virginia Tech. Using simple yet amenable compounds to give a basis (using MATLAB, students write their own code to display asymmetric units and the atoms within), students then work up to a more complex compound of their choice. All in all, a diverse and fascinating session. *Helen Walden*



Scenes from the opening reception at Newport Aquarium. Top left: Christine Muchmore with the shark; Michael Blum and, behind him, Arno Lentfer, talking to Janet Newman and an unknown crystallographer with his back turned.

Middle: Crystallographers in the fishy "tunnel," and, on the right, Ana Vivas not too sure about petting a turtle.

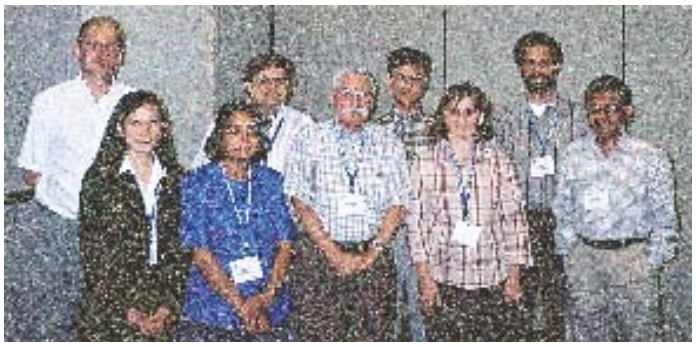
Bottom row from left: Jeff Deschamps, Kay Onan, Frank Allen, Helen Berman and George Phillips.

6.01: Structure Determination from Powder Diffraction

The first session organized by the newly formed Structure Determination from Powder Diffraction (SDPD) Special Interest Group, (*a.k.a.* Powder S1G) featured eight papers divided into two broad areas of research: results on how the structures were determined and experimental techniques with existing instrumentation.

The first presentation was by **Manju Rajeswaran** who described efforts to structurally characterize a microcrystalline polymorph of n-(p-tolyl)-dodecyl sulfonamide. She used synchrotron powder data with Monte Carlo procedures, coupled with quantum mechanical calculations and solid state NMR to solve and validate the structure. **Naima Bestaoui** discussed structural characterization of pillared cadmium and zinc amino-phosphonates; the difficulties presented by pseudo symmetry issues and means to get around these difficulties. **Peter Zavalij** presented a review of recent work on the power of structure determination from powder diffraction in materials science research, in the context of lithium battery components and related materials. Due to this breadth, this presentation illustrated the multitude of paths available in SDPD work. **Xiang ("Sean") Ouyang** described recent work in the Zn/S/diamine system from powder data, with an excellent overview of several techniques required for structure solution.

Felicitas Bidlack described phase characterization and extent of biomineralization of tooth enamel using thin sections of teeth, rather than ground material, using an instrument designed for both single crystal and powder work. **Bryan Chakoumakos** described attempts at solution of a low temperature phase of $K_2V_3O_8$. It was proposed that the phase



In back, l to r: Peter Zavalij, Kingsley Smith, Sean Ouyang and Brian Chakoumakos; front row: Cikui Liang, Manju Rajeswaran; Abraham Clearfield, Naima Bestaoui and Nattamai Bhuvanesh.

transition involves small displacements of vanadate and vanadyl polyhedra, and approaches using Distance Least Squares refinements were discussed. **Nattamai Bhuvanesh** illustrated methods to collect data from microgram sized samples, such as are frequently available from forensic studies, artwork characterization and archaeological work. The method involved mounting of the specimen in a small (0.1mm) nylon loop of the type frequently employed by macromolecular crystallographers. **Kingsley Smith** described how a crystallographer equipped with a current area detector diffractometer designed for single crystal work could be used for collection of powder diffraction data, and software packages developed by one of the main instrument manufacturers for the purpose. Finally, **Cikui Linang** showed results from a new algorithm developed to index powder patterns of unusual unit cells (e.g.,unusually flat or long unit cells) as programmed into a widely used commercial suite of materials science programs.

In the first business meeting of the Powder SIG a slate of officers was nominated with elections to be held in the near future. Interested ACA members are invited to affiliate with this SIG.

Abe Clearfield and Alex Yokochi.

8.01: Probing the Frontier of Soft Condensed Matter Science with Small Angle Scattering

This session highlighted the unique and important role of Small Angle Scattering in soft condensed matter science research. The session was chaired by **Elena Kondrashkina**. **Susan Krueger** from NIST opened the session with an overview and recent examples on Small Angle Neutron Scattering studies on biological systems. Combined with H/D isotopic substitution, SANS is extremely effective in studying structure-function relationships of proteins, such as conformational changes of proteins upon ligand binding. **Jaby Jacob** from Argonne reported their time-resolved synchrotron Small Angle X-ray Scattering studies on protein folding. Results on ubiquitin and the common type acylphosphatase refolding under changing denaturing conditions were reported. **Charlie Glinka** from NIST demonstrated yet another aspect of SANS's potential, the study organoclays. By using SANS, the researchers were able to gain insights into the interactions between the organically modified clay platelets and organic solvents, a key information needed in synthesizing organoclay and polymer nanocomposites. **Frederico Ferreira** and **Hamilton Napolitano**, both from the University of Sao Paulo, Brazil, and both recipients of this year's SAS SIG's travel award, each presented their SAXS works on protein systems. Ferreira showed the remarkable homology models that one can obtain from SAXS data. Napolitano presented a systematic evaluation of using SAXS to determine the molecular weight of the scattering protein particles, and hence the aggregation state of the proteins under study.

Jinqui Zhao

Newport Aquarium photo by Judith Flippen-Anderson

9.01: Important Science From Small Molecule Structures

The Small Molecule SIG put its science up front in a three-session program which combined talks by chemists whose structures have led to important findings, talks by crystallographers who use structures for discovery, and presentations on enhancements expected to result from new developments in technique.

The program was launched by **Carlos Murillo** (Texas A&M), who described the structures and the amazing associated redox properties of a series of dimetal complexes with the "hpp" ligand. The compounds include the $W_2(hpp)_4$ molecule, which has a first ionization potential lower than that of cesium metal. The hpp ligand has allowed the synthesis of dimetal units of other metals having heretofore unknown oxidation states. The perfect correspondence between the bond orders and the expected bond distances *vs* crystallographic results was appreciated.

Charles Simmons (U. Hawaii at Hilo) described very nice experiments in which the Jahn-Teller distortions in $[M(H_2O)_6]n^+$ complexes were probed, and provided convincing examples of the confirmation of theory by means of crystallography. The directions of the J-T distortions can be switched with applications of various combinations of temperature and pressure. **Art Schultz** (Argonne) continued the discussion of Jahn-Teller distortions in $[M(H_2O)_6]n^+$ complexes, adding the experiments in which the identity of the cation is changed. Art complemented the pressure and temperature studies with the addition of H-isotope effects. **Mike Hursthouse** (U. Southampton) provided current and future strategies for dealing with the explosion of data, and promoted the recording of even more data related to the environment of every experiment (including the recording of seemingly irrelevant environmental factors). His suggestion that "more data are needed" was backed up by the fact that we still can't predict crystal structures. Mike promoted the expansion of the fully automated laboratory, to enhance advanced data mining techniques that allow more comprehensive pattern searching. He suggested that we need to separate the data from the ideas, and to make all data available in accessible archives while continuing to distribute ideas via publication.

Ronald See (Indiana U., PA) presented the relative merits of hybridization (not physically realistic), VSEPR (realistic but hard to quantify), and Ligand Close Packing (LCP, quantifiable and physically realistic) theories for modeling AX_3E and AX_2E_2 coordination compounds. LCP predictions were compared to the results from molecular mechanics and from advanced calculations, and Ron showed how LCP can be used to improve the molecular mechanics model. **Scott Speakman** (ORNL) introduced a remarkably practical use of crystallography in studies to determine the causes of low light output from crystalline Lu_2SiO_5 (LSO). Both low and high-light-output LSO have the same lattice parameters and thermal behavior. Twinning is observed in some low-output samples, and others display dramatic peak broadening. Annealing has been found to return low-output LSO to a high-light-output state; Scott is preparing to do more beamline studies on these samples. Also, TEM has revealed some defects and inclusions in low-output samples, suggesting additional studies.

9.01-am: from left in back, Mike Hursthouse, Scott Speakman, Charles Simmons, Richard Cooper, in front: Arthur Shultz, Carlos Murillo, Ronald See, Lee Daniels

Richard Cooper (U. Oxford) topped off the morning session with a whirlwind trip through the problems presented by $Z'>1$ structures. These systems may occur when more than one conformation of a molecule is present, and often are beset with pseudo-symmetry and non-crystallographic symmetry. They may also raise eyebrows when there is a suspicion that the true symmetry has been missed. Correlation may be a problem during refinement, so restraints, reparameterization of the normal matrix, and eigenvalue filtering may be helpful. Richard suggests combining all three of these techniques for satisfactory structure refinement. Richard may have set a new record for the number of slides per minute!

The second session in the program, ably presented by **Allen Oliver**, had a distinctly inorganic chemistry flavor. **Ahmed Mohamed** of

9.01 -pm: from left, Xiang Hao, Alberto Albinati, Thomas Koetzle, Lothar Stohl, Karl Seff, Ahmed Mohamed, Allen Oliver

Texas A&M kicked off the session with a talk on gold chemistry, in which he described the pi-acid/pi-base behavior of trinuclear Au(I) complexes with pi-electrophiles. Pi acid-base interactions were identified in studies involving the gold-containing substrate with various organic entities, including TCNQ and octafluoronaphthalene. The acid-base character of the components was further clarified by DFT calculations, but the structural features of the products provided the bulk of the results. **Karl Seff** gave a talk on the eye-opening formation of at least four new ions produced by the disproportionation of elemental sulfur and iodine when they are sorbed into zeolite X, when the latter has been dehydrated and Cd-exchanged. The new ions, all the more surprising because of the paucity of previously demonstrated elemental disproportionations, are stabilized by the entities present in the zeolite framework - the new anion by interaction with Cd_2^+ and the cations in the oxygen-rich zeolite rings and cavities. **Lothar Stahl** continued the program with a description of yet another rare chemical species, a phosphorus-nitrogen triple bond produced in his ligand-design studies. The triple bond was characterized principally by its struc-

tural properties, which place the P-N distance within the range of those observed for previously verified P-N triple bonds.

Two talks placed strong emphasis on neutron scattering, with a view to the foreseeable enhancements in the use of neutrons in chemistry when the Spallation Neutron Source (SNS) comes on line. **Tom Koetzle** (Argonne and Brookhaven) gave a talk on the importance of neutron-based structural studies in the area of transition-metal-based catalysis and hydrogen activation. He also gave a preview of the striking improvements that are expected when the Single Crystal Diffractometer at SNS becomes operational, possibly within several years. **Alberto Albinati** (U. Milan) discussed the importance of neutron scattering in characterizing metal hydrides and extended the description of the chemically important applications of neutrons to the characterization of dynamics in hydrides through the use of inelastic neutron scattering (INS). Adding DFT calculations to the repertoire, Alberto showed how this combination of techniques could be used to extract a description of rotational barriers and hydrogen/hydride exchange involving transition metal complexes.

Evgeny Dikarev (SUNY Albany) described the disproportionation of diruthenium(II,III) trifluoroacetate to give Ru_2(II,II) tetrakis(trifluoroacetate) and the trimeric Ru_3(II,III,III) oxo-trifluoroacetate. His structural studies show that the trinuclear compound is valence-detrapped down to 213 K, and imply that a destructive transition at lower temperatures may be caused by a switch to a valence-trapped state. The final speaker of the Sunday afternoon session, **Xiang Hao** (U. Kentucky), described a thorough characterization of a copper crown ether complex that undergoes a first-order, but reversible, phase transformation at 315-320 K. The phase below the transition has a modulated structure. A parametric study (cell dimensions vs. temperature) over a wider temperature range was complemented by differential scanning calorimetry, which confirmed the phase transition.

The third part of program focused largely on questions of supramolecular assembly and whole crystal structures as opposed to questions of molecular structure. Attendees heard talks covering topics in crystal engineering, structural polymorphism, structure-property relationships of crystalline materials, factors influencing crystallization, and structural phase transitions. **Christer Aakeröy**, Kansas State U., started the morning with a discussion of his group's work towards rational synthesis of supramolecular assemblies. He described work on binary co-crystals that demonstrated the principle that the best hydrogen bond donors seek out the best hydrogen bond acceptors, and laid out plans for using molecules as interchangeable modules for building structures with predictable connectivity. He concluded with an example of a ternary co-crystal constructed according to his approach. **Tatiana Timofeeva**, New Mexico Highlands U. Dept. of Natural Sciences, presented work focused on investigation of polymorphs and polytypes of polar organic compounds. She offered an impressive suite of analytical and theoretical results with a theme of understanding and ultimately predicting crystal structures and habits. **Sean Parkin**, U. Kentucky, followed with a description of molecular packing motifs in various functionalized acenes, and how the solid-state (crystal and thin film) structures correlate to electronic properties. Analysis of the structures coupled with property measurements has allowed the group to tune solid-state electronic properties by adjusting the functional groups of the acene molecules, leading to a wide range of possibilities for constructing real-world devices. **Gary Enright** presented results on several varieties of structures of *t*-butylcalix[4]arene co-crystals with fluorinated benzenes. Both steric and electronic effects appear to be important in determining the orientations of various fluorobenzene guest molecules inside calixarene cavities, and indeed whether particular fluorobenzenes occupy the internal cavities at all. In addition to common tetragonal structure motifs, some distorted motifs involving correlation between guest positions in adjacent hosts were reported, as well as one structure in which the fluorobenzene resides in the interstices between the calixarene molecules instead of in their cavities.

Carolyn Brock, U. Kentucky, provided an enlightening discussion of fractional crystallization, co-crystallization, and solid solution formation. She observed that when the opportunity for co-crystallization or solid solution formation is present, the crystalline product(s) obtained depend on the molar ratios of the components present in the crystallization mixture, and that the ratio that leads to the greatest yield of the desired solid-state product may be far from the ratio in the product. True solid-state co-crystals other than solvates are rare, Carol pointed out, and a significant proportion of those that have been observed are quasiracemates. **Alicia Beatty**, U. Notre Dame, presented a paper on structures of organic clay mimics - compounds exhibiting a layered structural motif analogous to that of clays. The study described involved use of different alkylammonium cations to attempt to engineer desired properties into the interlayer space of the target structures. **Frank Fronczek**, Louisiana State U., continued the session with a paper on the polymorphs of D-mannitol. D-mannitol exhibits several accessible structural polymorphs, but the structural details of the one of most interest for pharmaceutical use had not previously been published. Frank reported a structure of this "δ" polymorph consistent with previous unit cell and space group reports, and based on that structure argued that the previously reported α polymorph is in fact the same as the δ polymorph. Pseudosymmetry of the structure of the latter likely explains the different crystal system and space group with which the former is described in the literature. **Carl Schwalbe**, Aston U. Pharmacy School, closed the session with a discussion of close hydrogen - hydrogen contacts in the structures of certain amidrazone derivatives. The presence of such contacts varies with the derivative. In two cases the close contacts predicted based on the geometry of the nonhydrogen atoms are consistent with crystallographic refinement of the hydrogen atom positions, but in a third case the refined positions are quite different, separated by almost the sum of the *van der Waals* radii, and this separation is consistent with *ab initio* molecular orbital optimization.

In organizing the program on *Important Science from Small Molecule Structures*, the Small Molecule SIG set out to display the rich and significant science derived from small molecule structures. The enthusiastic participation of chemists and crystallographers alike, along with the results themselves, gave the attendees a good taste of the wide-ranging and important science inherent in these structures.

Larry Falvello and Lee Daniels

10.01: Synchrotron and Neutron Diffraction Facilities Posters

This evening session was well attended, given this was the first time that a display exclusively for synchrotron and neutron facilities had been organized. Authors from 25 experimental facilities covering a dozen national and international laboratories show-cased the capabilities of their particular experiments. The **Advanced Photon Source (APS),** (*see images, opposite*), and the **Intense Spallation Ion Source (ISIS)** were both well represented, sharing nearly half the posters in the presentation.

Topics that were presented ranged from microcrystal small molecule diffraction experiments to protein and macromolecular data collection to neutron powder and neutron single crystal diffraction services. Several of these facilities offer specilialized services for unusual samples, while others are capable of bulk data collection. Protein and macromolecular facilities had the largest showing, with eight posters. Neutron sources were also very well represented; with both existing laboratories [ISIS, the **Intense Pulsed Neutron Source (IPNS)** and **Insitut Laue-Langevin (ILL)**] and laboratories in production [**Spallation Neutron Source** (**SNS)**] displaying posters. The additional presentation tables were well utilized and, in one case, covered with material from the **Los Alamos National Laboratory (LANL)** and the wide variety of services offered there. It appeared that interest amongst the crystallographic community was incited. There were many discussions between the authors and parties interested in what the various facilities had to offer. The authors were more than willing to discuss the benefits (and in one case, cautionary tales) of their particular facilties. It is likely that with such show-casings the facilities will see an increase in patronage as the (sometimes hidden) benefits of such experiments are presented to the wider community. Look for further similar sessions at future ACA meetings if you missed the Synchrotron and Neutron Sources Facilities Poster Session this year.

Allen Oliver

11.01: Topics for the Young Scientist

This session was organized and designed to aid the next generation of crystallographers. While the technology and areas of research change all the time, the development of young scientists consistently remains a crucial aspect of the scientific community. Have no doubt about it, with over 150 attendees at the YSSIG session, the young scientist is a contributing factor in today's science.

Joel Shulman recently retired from P&G kicked off our session with an outstanding talk on interviewing skills. Joel, now at the U. Cincinnati teaches a class for 3rd and 4th year graduate students entitled "*Life After Graduate School*". In addition Joel gives workshops to the ACS Dept. of Career Services. **Brenda Schulman,** a new faculty member at St. Judes, followed Joels talk with some personal highlights of her career. Brenda, still being a "young scientist" in the eyes of the ACA, was able to give good advice to all in attendance. **Howard Einspahr** is a long time crystallographer who gave his opinion on the current state of the job market for young scientists. Howard's talk put it in black and white so to speak, and generated much debate in the background.

Vivian Cody, **Bob Sweet**, **Jon Clardy**, and **Steve Ealick** formed a panel to discuss grant writing. The panel began by explaining the types of funding available and how to go about receiving funds. Although most of the discussion was biased towards NIH and DOE funding the panel did a great job in lending advice from years of experience. The restructuring of NIH's funding mechanism was also described to some extent, based on the knowledge of the panel. The discussion continued for some time and was well received by most. **David Rose**, the Canadian Representative to the ACA Council, was in the audience and contrasted U.S. and Canadian funding systems.

C. Kent Brown

"Chemical" Posters

The "Expo" at the Covington Convention Center housed the posters for a variety of topics, one of which was rather inauspiciously named "Chemistry." Like frogs in a dynamite pond,[1] these posters could be found scattered about amongst the riff raff. The topics were rather diverse, and the highlights are grouped below according to some common chemical categories:

Organic chemistry: P014, *Molecular Interactions and Methanesulfonanilides*, an offering from **Penelope Codding and Paula Lario**, (U. Victoria; U. British Columbia), in which it was shown how intramolecular interactions such as sterics between a phenyl group and the NH group, in combination with a proposed CH-O hydrogen bond, limits the possibilities for intermolecular interactions.

Inorganic chemistry: P016, *High Pressure Structural Studies of* $Ru_3(CO)_{12}$ by **Carla Slebodnick** and coworkers (Virginia Polytechnic Institute; State U., Blacksburg, Virginia), in which the effect of high pressure on the geometry of the title compound was investigated. In this case, while intermolecular distances were found to decrease with an increase in pressure, the geometry of the cluster did not change significantly up to 8 GPa.

Computation: Two posters were given on new applications for databases. One, P023, **Camden Hubbard**, ORNL, and collaborators at ICDD, *PDF-4/OrganicsNew Content in a Relational Database Format with Integrated Search and Retrieval* outlined the addition of calculated powder patterns from structures published in the CSD to the Powder Diffraction File. The second P060,was given by **Zukang Feng** et al, PDB at Rutgers, *LigandDepot: An Information Resource for Small Molecules*, described an interface for finding small molecule information for those interested in binding to proteins and nucleic acids.

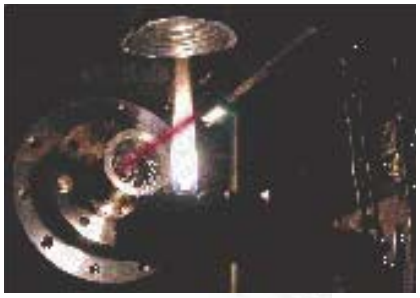
Medicinal: P047, *Experimental Determination of the Charge Density of Mesulergine, A Dopamine Agonist*, **Cheryl Klein Stevens** et al, Xavier U. of LA; U. of New Orleans) gave a view of how charge density studies are being used in disease-related research *(see figure,opposite page).*

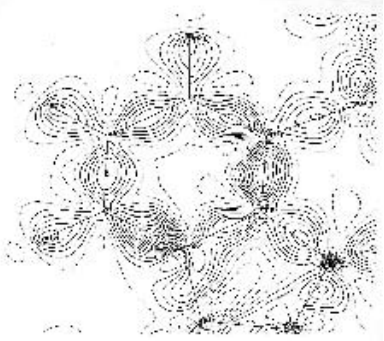
[1]My apologies to John Steinbeck and the characters in Cannery Row.

Alicia Beatty

Poster 10.01.10: from Steve Ginell, SBC (Structural Biology Center at Argonne) sector 19 ID beamline experimental hutch, and Kappa Goniostate located there.

8.02 images from Gregory Beaucage: nano-particle (silica) generating flame in the pinhole SAXS camera at ESRF HBBL (Narayanan). SAXS yields, particle density, size, and aggregate structure as a function of position in the flame. These data are used to verify simulations of particle growth and particle growth models in flames. 1cm height above burner corresponds to about 10 milliseconds in this continuous process; flame temperature is about 1500 centigrade at the base of the flame.





From Cheryl Klein: A map of the electron deformation density plotted in the plane of the aromatic ring in mesulergine hydrochloride, a dopamine agonist, shows the distribution of electrondensity in the covalent bonds. Contours are drawn at 0.10 e/A3.

12.01 - 12.03: Biomacromolecular Crystallization.

Three sessions on this subject were organized by the American Association of Crystal Growth in cooperation with NASA: ***Biomacromolecular Solutions, Phase Separation and Nucleation***, with the program compiled by N. Asherie, ***Biomolecular Crystal Growth and Perfection*** by Robert Thorne and ***Crystal Engineering, New Techniques and New Crystals*** by Cheryl Janson, with help from A.A.Chernov. The sessions were well attended and added to our knowledge and understanding of solutions from which crystals grow, the growth processes themselves, biomacromolecular crystal properties, freezing processes and practical crystallization approaches. The ultimate goal pursued by these sessions, also held at earlier ACA meetings, is to bring more scientific rationale to protein crystallization and to better understand the general behavior of complex biomacromolecular systems, liquid and solid.

12.01: Biomacromolecular solutions, Phase Separation & Nucleation.

Seth Fraden presented light scattering measurements of the second virial coefficient for lysozyme in presence of PEG in solution, and also aspects of thermodynamic theory, including second and third virial coefficients. Unlike findings with other proteins, addition of PEG to the reported solutions results in a repulsive interaction between proteins, whereas entropic effects usually cause inert polymers to produce "depletion" attraction between lysozyme molecules. Neither does the second virial coefficient crystallization slot concept work in this case. Static and dynamic light scattering were also applied by **Peter Vekilov** et al. to ferritin and apoferritin solution to study intermolecular forces. Hydrated Na^+ ions between two negatively charged macromolecules seems to be responsible for repulsion forces at distances exceeding hydrated Na^+ cluster size while Cd^{2+}, known to make Cd - ferritin crystalline salt, induces attraction at small distances. MC simulation with non-monotonous intermacromolecular potential have been reported to explain lack of liquid-liquid phase separation and temperature dependence of ferritin solubility. Initial stages of liquid-liquid phase separation in lysozyme solution was put forward by **Marc Pusey** as a reason for the earlier found decrease of the crystal growth rate with increasing supersaturation. He also presented structural arguments for clustering of lysozyme molecules into tetramers.

Alice Gast spoke on 2-dimensional streptavidin crystals growing on the biotinylated lipid monolayers on water surfaces and on bilayer vesicles. Variation of pH, $4 < pH < 7$, and of ionic strength resulted in morphologies varying from single faceted 2D crystals to dendrite-like, S-like shapes as well as those resembling split polymer crystal aggregates. Point mutations change crystal structure. The protein crystals grown on a vesicle surface visibly modify reaction of the vesicle to external force, i.e. the elastic properties of the vesicle membrane, and may even completely prevent elastic relaxation of a vesicle: vesicles initially partly soaked into a capillary and then released were not deformed. **Werner Kuhlbrandt** and **Michael Wiener** reviewed principles and techniques to grow membrane proteins in two and three dimensions, respectively. Werner reported that 2D crystallization of the plasma membrane of ATPase and c-subunit ring of the ATP synthase crystals were obtained by detergent dialysis. The crystals allowed ~6-8 Å resolution by electron diffraction. The ordered molecules in the crystal are supposed to be connected by their hydrophobic parts via the detergent molecules aligned along these parts. Michael discussed the development of detergent specific crystallization screens for membrane proteins.

Alex Chernov

High Pressure Science

June 4-15, 2003, Erice, Italy

118 participants convened at the E. Majorana Centre for Scientific Culture, Erice, Italy for the 34th Course organized since 1974 by the *International School of Crystallography*, one of the more than one hundred cultural sections of the Centre.

This was the first such course dedicated to high pressure research and highlighted the progress, interdisciplinary aspects, and the bright future of high pressure science. Based upon the very high score given to the course by the participants (all Erice courses are scored), this is likely to be first of many similar summer schools on high pressure science. The success of the scientific sessions and the extra curricular activities can be traced directly to the tremendous efforts of the local organizers, the Executive Secretary **Paola Spadon** and the Treasurer **Lodovico Riva di Sanseverino**. They, Course Directors **Andrzej Katrusiak** and **Paul McMillan**, and the dedicated staff made an enjoyable scientific school into a memorable experience. Erice, an incredibly beautiful and peaceful setting in any circumstance, was made all the more attractive by fine food, excellent local entertainment, and excursions to nearby archaeological sites.

The Course covered a wide range of sub-disciplines: solid state physics; organic and solid-state chemistry; geophysics and molecular biology. Several workshops concentrated on techniques, "best practice" and hands-on demonstrations of computer programs. Invited lectures were punctuated by active discussion, and the two poster sessions were also lively affairs, and were preceded by an equally lively and enjoyable series of 1-minute presentations by poster presenters. This session was chaired by **Malcolm McMahon** who later expressed surprise and even some disappointment at not having to wield "the bell" to encourage presenters to keep to time.

In all, 88 selected participants from 21 nations were addressed by 30 invited speakers. This was the first time that an Erice meeting was broadcast live on the web, thanks to considerable effort on the part of the in-house computer staff, led by John Irwin. Remote participants from countries around the world posed questions to speakers via the electronic chat room.

The speaker list included leaders in the high pressure field who described techniques and recent developments, as well as giving insights into where the field is heading. The meeting began and ended with inspiring lectures by directors **McMillan** (solid state chemistry at high pressure) and **Katrusiak** (thermodynamics of structural transformations in hydrogen-bonded substances). The fundamentals of static and dynamic high pressure techniques were covered by several speakers including **Batsanov** (shock waves), **Shimomura** (studies using large volume devices at synchrotron sources, especially in Japan), **Pasternak** (diamond anvil cells, Mössbauer and magnetic studies), and **Mezouar** (high pressure synchrotron studies at the ESRF). **Szafranski** discussed phase transitions by high pressure dielectric spectroscopy and calorimetry. A lecture by **Dubrovinsky** dealt with techniques of high pressure crystallography at elevated temperatures as a fundamental tool for understanding materials deep within the earth. The power of modern theoretical methods and the insight into high pressure phenomena and the predictive capability they provide were highlighted in several lectures by **Oganov, Parrinello, Tse** and **Winkler.** Fundamentals of equations of state and their accurate determinations were discussed by **Holzapfel and Angel**.

Whole new classes of experiments are being carried out at high pressures, thanks to the increasing availability of synchrotron x-ray and neutron sources at international facilities, improved methodologies, and better area detectors. The possibilities for new, more accurate and more precise science at these facilities were emphasized in lectures by **Hausermann** (the new APS high pressure facilities) and **Angel** (more accurate data from diamond anvil cells in the laboratory environment), **McMahon** (accurate data from powders, single crystals, "poor" single crystals, and various combinations of these), **Itie** (x-ray absorption spectroscopy at extreme conditions) and **Parise** (mapping changes in atomic structure using powder diffraction data).

Emerging fields included studies of the effects of pressure on organic materials, addressed by **Boldyreva** and macromolecular crystallography and other "soft" materials at high pressures, covered by **Gruner** and **Fourme**. The recently discovered modulated structures of "simple" elements were discussed by **McMahon**, their treatment was addressed by **Petricek**, and possible reasons for their formation and stability were given by **Degtyareva**. Specific topical areas where the power of high pressure techniques to provide unique structural information under the "operating conditions" of important materials included lectures by **Kuhs** (high-pressure clathrates), **Loveday** (neutron diffraction studies of ices and ice mixtures), **Pusztai** (structural studies of high-density forms of amorphous ice), **Solozhenko** (*in situ* studies on the synthesis of superhard materials), and **Goncharenko** (magnetic properties of crystals and their studies at high pressure conditions). Not all high pressure crystallography is necessarily done *in situ*. Three speakers emphasized materials synthesized at high pressures and recovered to room pressure conditions. These included presentations by **Ross** (bonding of charge balancing cations in framework stabilized at high pressure), **Gauzzi** (cuprate superconductors prepared under high pressure) and **Armigliato** (analysis of localized strains by convergent beam electron diffraction)

Copies of the lecture presentations will be posted on the web at **http://erice2003.docking.org/**.

John Parise and Sol Gruner

Gordon Research Conference (GRC) on Proteins, June 22-27, 2003

This Gordon Conference meets every two years at Holderness School in Plymouth, New Hampshire. The 122 participants included a good representation of academic PIs (50%) and graduate students/postdocs (30%), and there were also a number of participants from industry and government labs. An international flavor was provided by the 30% of participants from outside the US.

The meeting featured presentations on protein folding, structure design, protein-protein interactions, new methods, membrane proteins, proteins and disease, and protein machines. A major emphasis was given to alternative folds and misfolding, including amyloid diseases, topics that were discussed in the opening and closing keynote addresses given by **David Eisenberg** and **Chris Dobson**. Each of these presentations gave overviews and discussed large bodies of data, yet succeeded in clarifying the field by emphasizing underlying principles. The four full days of the conference were filled, in usual GRC style, with 30 minute and shorter talks in the mornings and evenings, posters in the afternoons, and plenty of time to discuss science informally while biking, hiking, playing a variety of casual sports, or socializing in the bar.

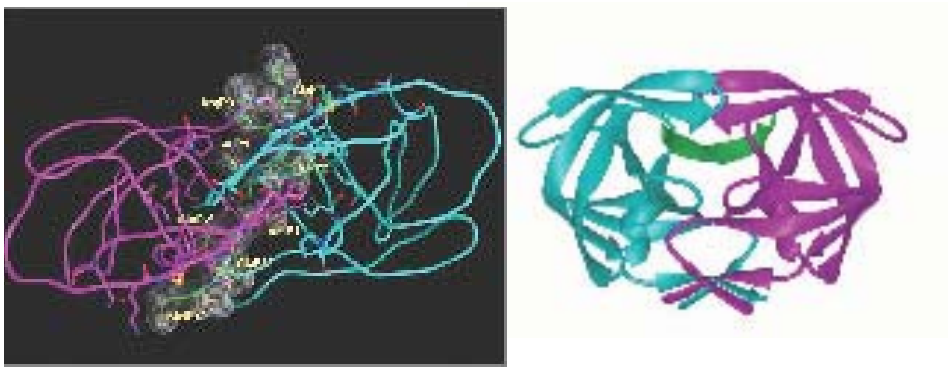
Rather than mentioning individually each of the 34 talks presented, I will briefly discuss a few general points that emerged during the meeting. I hope that the many excellent speakers and poster presenters not mentioned here explicitly will forgive the highly restricted scope of this review, which is forced by space limitations. The session on membrane proteins was a reminder that this is a frontier topic that in almost every way is in its infancy in comparison with globular proteins. Except, perhaps, that the prediction of membrane protein structure may be an inherently simpler problem than that of globular proteins. This is because the vast majority of membrane proteins are helical and because the helices are stable and essentially fully formed when the protein is unfolded in the membrane. Consequently, folding of many membrane proteins is, to a first approximation, a matter of docking preformed helices.

Charles Deber and **James Bowie** provided mixed results on the importance of hydrogen bonds for membrane proteins. Because of the hydrophobic environment, these electrostatic interactions are inherently very strong in the membrane and in some cases can dictate oligomerization state. In other cases, however, hydrogen bonds apparently provide no more stabilization than corresponding *van der Waals* interactions. This surprising result may reflect the geometric constraints on optimal hydrogen bond strength and the submaximal stability of many membrane proteins. Evolution, of course, only cares about stability to the extent that it impacts function, and because many membrane proteins have a highly restricted unfolded state (preformed helices), they have the potential to attain far greater stability than required, or even desired, by natural selection. This conclusion is supported by the observation that, in contrast to globular proteins, random mutations have a relatively high probability of stabilizing membrane protein structure.

Several successful protein design projects were testament to the fact that design is easier than *de novo* prediction. This follows from the long established observation that quite different sequences can adopt the same three-dimensional structure, and fuels efforts at prediction by homology modeling and threading. In contrast, however, **Angela Gronenborn** described the case of the small protein GB1, which she calls a protein contortionist because substitution of one or a few amino acid residues resulted in two dramatically refolded structures. This illustrated the ability of proteins to explore conformational space during evolution and also sounded an interesting caveat to the general rule that similar sequences encode similar structures.

Jim Wells described the "tethering" approach to identification of inhibitors of protein-protein interactions. One finding from this work was that the majority of ligands identified bound to regions of the protein surface that could assume multiple conformations. This contradicts the expectation that entropic effects favor binding to preformed surfaces, but is explained by the "more shots on goal" hypothesis. In another disease-related talk that drew heavily upon crystallographic data, **Celia Schiffer** described development of new HIV protease inhibitors that will be guided by analysis of structural envelopes for various substrates and inhibitors. The key realization in this effort was that drug resistant mutations can arise only if the mutation does not significantly disrupt an important interaction with substrate. Thus, inhibitors are less likely to suffer drug resistance if they are relatively small and only contact protein groups that are required for substrate binding.

Examples of the importance of conformational changes in protein function were provided in the final session on protein assemblies/proteins in action. These included protein complexes



From Celia Schiffer: Crystal structure of the capsid-p2 substrate complexed with an inactivated (D25N) HIV-1 protease. Similar figures were published in: Prabu-Jeyabalan, M., Nalivaika, E.A., King, N.M., Schiffer, C.A. , *J. Virology* (2003), 77(2), 1306-15; Prabu-Jeyabalan, M.M. et al, *Structure* (2002), 10(3) 369-38; and Prabu-Jeyabalan, M.M., Nalivaika, E., Schiffer, C.A., *J. Mol. Biol.* (2000), 301(5), 1207-20.

Gordon Conference on Proteins, con't

switching between active and inactive states, new insight into the allosteric mechanism of heamoglobin (**Gary Ackers**), and kinetic and electron microscopic studies on molecular motors (**Enrique De La Cruz** and **Stan Burgess**). Clearly, the relationship between protein structure, conformational changes, and function, deserves continuing emphasis at future meetings.

The role of protein misfolding in various diseases was discussed in several talks, including the presentation by **Jeff Kelly**, which surveyed the various ways in which proteins misfold. In addition to simply failing to fold, these defects can include failure to achieve correct intracellular location, recognition by cellular degradation machinery, and formation of the infinite beta structures of amyloid deposits. One particularly interesting example of progress toward developing therapeutics included use of an enzyme inhibitor to stabilize the enzyme fold during trafficking to the lysozome. This "chemical chaperone" does not significantly impair enzyme function because substrate concentration is high in lysozomes. In another example, a ligand was developed to stabilize the tetrameric form of a protein, after it was realized from kinetic analysis that aggregation proceeds via disassembly of the tetramer to a monomeric state.

A familiar but important message for crystallographers from the meeting was that structure determination should be integrated into boarder programs of research. Thus, the more than 10 talks that heavily featured crystallographic studies all incorporated significant contributions from other approaches, including spectroscopy, NMR, electron microscopy, chemical synthesis, enzymology, kinetic and thermodynamic measurements, cell biology, and computational methods. With this in mind, it should be noted that the session on new methods included developments with MALDI mass spectrometry to measure protein stability (**Michael Fitzgerald**) and protein-protein interfaces (**Elizabeth Komives**), and genetic approaches to identifying oligomeric proteins (**Jim Hu**) and evolving new protein functionality (**Virginia Cornish**). Notably, many of the "new methods" talks featured genome-wide capability. Clearly, even those of us that do not practice structural genomics must adapt to an era of high-throughput proteomics.

Although there were lots of excellent talks and posters, as always with Gordon Conferences, the major attraction was the opportunity to interact extensively with investigators and students in an environment that was scientifically intense and socially relaxed. This was possible because all participants stay on site and eat in the same dining room. Although boarding school dorms do not provide the height of luxury, and the humidity in a New England June is somewhat greater than some of the participants are accustomed to, the GRC format remains an excellent model for rewarding conferences. Finally, the GRC staff did an excellent job of making the meeting run smoothly, and the organizers, **Lynne Regan** and **Rachel Klevit**, are to be congratulated and thanked for putting together a very stimulating meeting.

Chris Hill

High Resolution Drug Design Meeting

Bischenberg-Strasbourg May 13 - 16, 2004.

The main purpose of this meeting is to describe the cases where high resolution x-ray crystallography has been used for rational drug design, and the latest methodological developments that allow such fine studies. Furthermore, a number of techniques such as mass spectrometry, microcalorimetry and NMR are highly complementary to the crystallographic studies, as they provide direct experimental evidence of binding energies. All this work needs theoretical modelling of the interactions. Therefore, the meeting also includes descriptions of these complementary techniques and of modelling efforts. International experts in each field will describe their work, with an emphasis on the synergy between different techniques to obtain useful information about ligand binding.

The Bischenberg Congress Center is located about 25 km from Strasbourg, in a beautiful place near the Vosges mountains. The registration fee, including food and lodging, is 500 Euros. The number of participants is limited to 100, and about 50 fellowships covering the meeting expenses will be available to young students. Details of this center can be found at **www.bischenberg.e-i.com/anaccu.htm.**

The deadline for applications for financial aid is February 1, 2004, and for all other registration is March 1, 2004. Details of the meeting, including the application form, will be available at **www-igbmc.u-strasbg.fr** after November 1st 2003. For further information, please contact **podjarny@titus.u-strasbg.fr.**

The diffraction of x-rays by molecular crystals is the technique of choice for obtaining three-dimensional information about atomic positions and interactions, information essential for comprehension of function and molecular mechanisms. In the case of biological macromolecules, the spatial arrangement of the components of proteins and nucleic acids can be correlated to their biological function. In particular, the x-ray determination of the structures of complexes of pharmaceutical targets with ligands is a powerful tool for identifying the molecular basis of potency and selectivity of potential drugs.

The resolution is an essential parameter of a crystallographic study. It is directly related to the minimum distance separating the details of the electronic density. A resolution of 2 Å is sufficient to distinguish peptides from a protein or the bases of a nucleic acid, but not the individual atoms, and even less the bond densities. At this resolution, the position and orientation of ligands in binding sites can be determined, but finer details, like protonation states and accurate interatomic distances, have to be imposed via stereochemical restraints.

In the last ten years, various technical improvements, ranging from better techniques of expression and crystallization to the use of synchrotron sources for measurements of diffraction and algorithms of multipolar and quantum modelling, have made it possible to improve considerably the resolution and the quality of the macromolecular models. Biological structural studies with resolutions between 1.5 and 0.9 Å have become more common. In this range of resolution, the individual atoms can be clearly distinguished and the hydrogen atoms start to appear. Interatomic distances can be determined with errors less than 0.01 Å, which enables accurate calculation of interaction energies and discrimination of single vs. double bonds. Estimation of the atomic charges starts to be possible.

Since 1997, several structures were solved with a resolution better than 0.9 Å, in particular crambin (Jelsch et al, (2000) *Proc. Natl. Acad. Sci.* U.S.A. **97**, 3171-3176), subtilisin (Kuhn et al, (1998) *Biochemistry* **37**, 13446- 13452) and aldose reductase (Podjarny et al, *Europhysics News* Vol. **33** No. 4, 113-117, 2002). With such a resolution, the level of the details observed in the best ordered areas approaches that of the small molecules studies. The hydrogen atoms and the bond densities are clearly visible, and the atomic errors of co-ordinates are reduced another order of magnitude (~0.003 Å), which makes the stereochemical differences highly significant. This level of detail enables a very fine description of the interaction between a potential drug and a pharmaceutical target, and the identification of the sources of potency and selectivity.

Confirmed speakers are: **Tom Blundell, Gerard Bricogne, Paula Fitzgerald, Richard Giege, Angela Gronenborn, Andrzej Joachimiak, Gerhard Klebe, John Ladbury, Claude Lecomte, Richard Pauptit, Alberto Podjarny, Andrea Schmidt, Thomas Schneider, Alain Van Dorsselaer, Irene Weber, Eric Westhof, Keith Wilson and Peter Zwart**.

Alberto Podjarny

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ACA 2004 July 17-22—Chicago, IL

The annual meeting of the ACA will be held in downtown Chicago at the Hyatt Regency Hotel on Wacker Drive. The hotel is located on the Chicago Riverwalk along the south side bank of the Chicago River adjacent to Michigan Avenue, nicknamed the "Magnificent Mile," and near Lake Michigan, Lake Shore Drive, and Grant Park. The conference and exhibition will be held in the East Tower of the hotel. The banquet will be in the Crystal Ballroom in the West Tower of the hotel, overlooking the Tribune and Wrigley buildings. Navy Pier, the Art Institute, the Field Museum, Shedd Aquarium, Adler Planetarium, and the Museum of Contemporary Art are all located nearby. Grant Park is the site for several summer festivals and concerts. Both airports, O'Hare and Midway, are located within twenty miles of the downtown area.

Chicago is home to several universities, and is a city of great restaurants, jazz and blues venues, museums, theaters, and sport's teams,

The Wrigley Building. Photo courtesy of Terry and Melody Howe, ChicagoPhotography.com.

2004 LOCAL CHAIRS

Karl Volz and Bernie Santasiero

2004 PROGRAM CHAIRS

Christer Aakeröy and Marilyn Yoder

Meeting Calendar

DECEMBER 2003

4-7 **High Pressure Structure and Reactivity: The Science of Change,** Lawrence Berkeley Nat'l Lab, Berkeley, CA

MAY 2004

13-16 **High Resolution Drug Design Meeting,** Bischenberg-Strasbourg, France, contact **podjarny@titus.u-strasbg.fr** *(see page 63)*

JUNE 2004

6-10 **American Conference on Neutron Scattering,** College Park, MD.

9-20 **Electron Crystallography: Novel approaches to Structure Determination of Nanosized Materials**, Erice, Italy

10-21 **Polymorphism : Solvates and Phase Relationships.** Erice, Italy. www.crystalerice.org

JULY 2004

17-22 **American Crystallographic AssociationAnnualMeeting,ACA 2004, Chicago, IL. Local Chairs: Bernie Santarsiero, bds@uic.edu; Karl Volz, kvolz@uic.edu; Program Chairs: Christer Aakeröy, aakeroy@ksu.edu; Marilyn Yoder, myoder@cctr .umkc.edu**

MAY JUNE 2005

28-2 **American Crystallographic Association Annual Meeting, ACA 2005, WALT DISNEY WORLD SWAN Hotel, Orlando, Fl. Local Chair: Khalil Abboud, abboud@chem.ufl.edu; Program Chair: Ed Collins, edward_collins@med.unc.edu**

AUGUST 2005

17-22 **XX IUCr Congress**, Florence, Italy. Local Chair: Paola Paoli, **iucr@iucr2005.it**, Program Chair, Carlo Meali, **www.iucr2005.it**

ACA 2005

Local Chair: Khalil Abboud, Dept. Chemistry, U. Florida; **abboud@chem.ufl.edu**

Program Chair: Ed Collins, Dept. Microbiology & Immunology, U. North Carolina, **edward_collins@med.unc.edu**

to be held May 28 - June 2, 2005 at the Walt Disney World Swan Hotel

Orlando, Florida