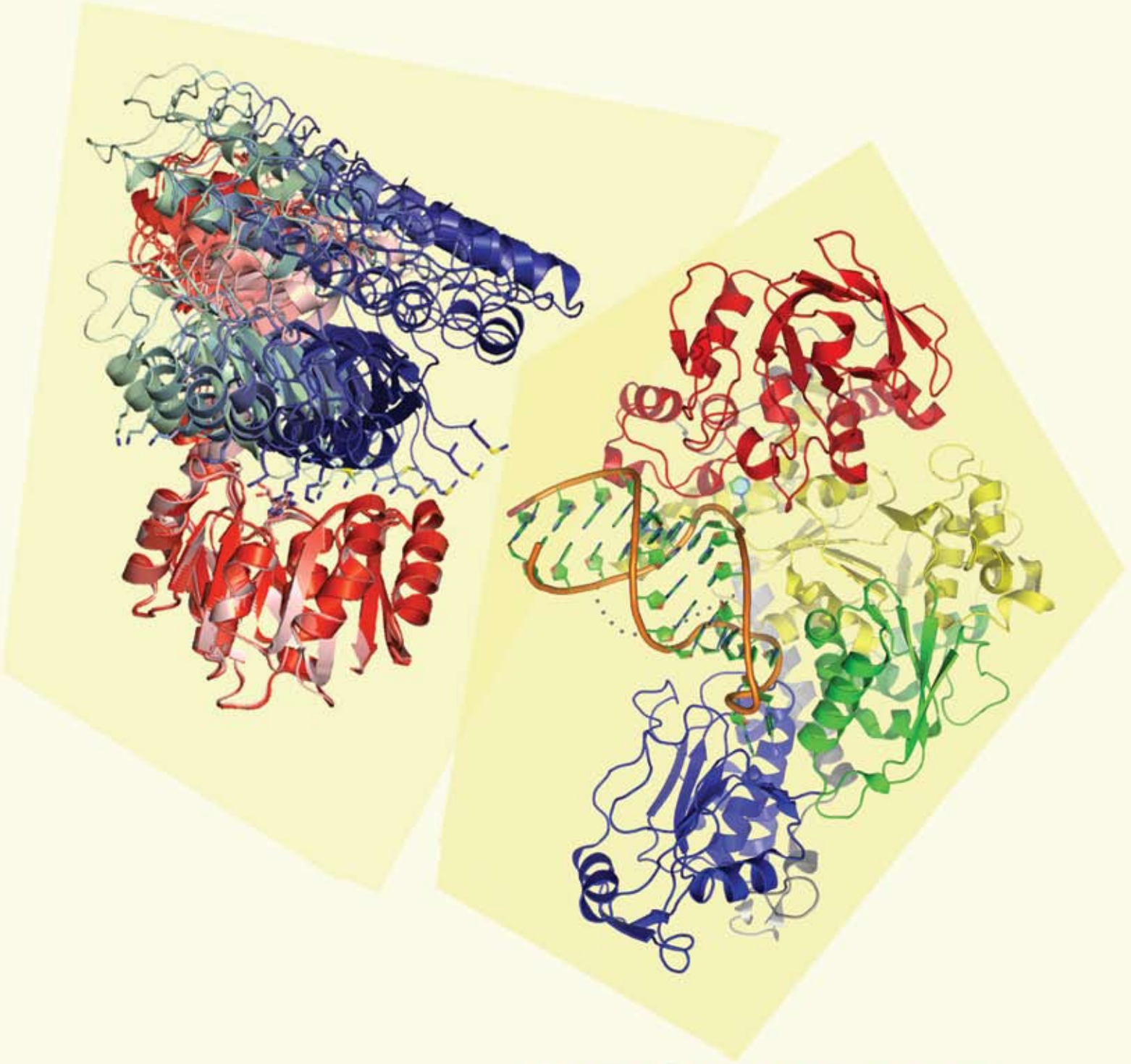
ACA RefleXions

American Crystallographic Association

Number 3
Fall, 2007



New Structures at the Salt Lake City ACA Meeting

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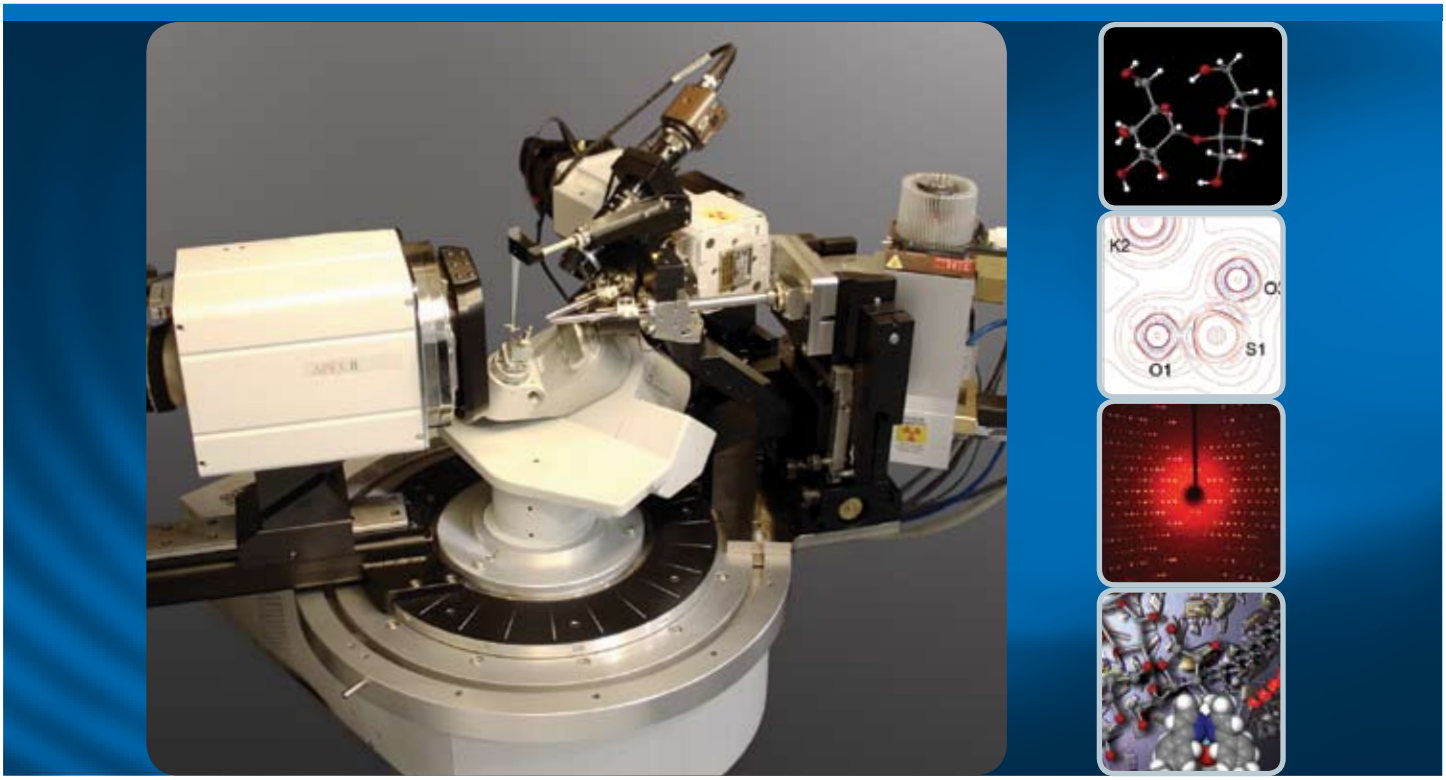

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Crystallography

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

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

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President's Column:

In this issue of RefleXions, I would like to begin by reflecting on the 2007 ACA meeting which took place in July in Salt Lake City. Reports of the various sessions are presented in detail in the rest of this issue. While visiting a number of the oral sessions, I made a very pleasing observation. This was a very balanced meeting, covering many aspects of our science. This was brought home to me by the observation that the attendance at some of the clearly non-macromolecular sessions was equally as good as in the macro- sessions. It has been a while since this has been the case, and was largely due to the efforts of the SIG leadership in choosing topics that could be sponsored by more than one SIG. This type of collaboration between the SIG's as well as ongoing discussions with the Denver Diffraction Conference concerning joint meetings of the two organizations is anticipated to generate even more exciting and dynamic meetings in the future. While on the topic of future meetings, I will remind you that because 2008 is an IUCr year, we will meet at the end of May in Knoxville (Paul Butler and Dean Myles, Program Chairs; Jason Hodges, Local Chair). Clearly the proximity to Oak Ridge National Lab should attract a significant number of members from the neutron community to this meeting, and planning for activities involving ORNL are well under way. Of course, a spring meeting means a tighter abstract deadline than in other years – December 15 - so please get this onto your "to do list."

At the business meeting in Hawaii, council was charged with the task of formulating a proposal to establish a fellows program for the ACA. This was suggested as a mechanism to recognize and honor those members of the ACA who have made major contributions to the discipline, and is a mechanism common to many learned societies. Accordingly, Council submitted a draft proposing a nomination procedure and extent of an ACA Fellows program to the members at the business meeting in Salt Lake City. In contrast to the response in Hawaii, council was soundly rebuked for wishing to establish a "class structure" into an egalitarian organization. Clearly two different subgroups of the membership were present at the two different meetings.

In this issue of *ACA RefleXions* there is a letter expressing dissatisfaction with certain aspects of our annual meetings. I thank the authors for making their opinions known, and hope that this will be the start of a dialog between council and the membership on issues that concern everyone. I would thus request of the membership two things; 1) if you have opinions on these or other topics, please make them known to council, either by email or by letters to *ACA RefleXions*; 2) please attend the business meetings so that a clear picture of the will of the membership emerges – this is your association and council is elected to represent your interests.

As a member of an organization that prides itself on the quality of the science carried out by its members, and the rigor inherent in the practice of crystallography, I was very disturbed by the recent controversy (see Janssen et al., *Nature*, 448, E1-E2 (2007) and related articles) regarding "fabricated" data. On the one hand, the idea of fabricating data is abhorrent to me. On the other hand, that criticism of the original paper should be censored by the editors of a scientific journal is highly unprofessional. However, I am proud of the fact that a large number of the crystallographic community were concerned enough to debate this issue electronically (CCP4BB). I am optimistic that there will eventually be a clear conclusion indicating whether this was an honest mistake, or dishonest behavior (perhaps there will be a discussion of the C3b structure at the Knoxville meeting?). This event should give pause for thought to those of us responsible for training scientists in the techniques of our discipline, and for instilling the concept of what is ethical, as well as to journal editors who must use the peer review process fairly and rigorously. As a final comment, faster may be better when looking for funding, but faster is rarely better in terms of the science reported.

Alan Pinkerton

Letters to the Editor

April 10, 2007

The occasion for this letter is the spring 2007 issue of *ACA RefleXions*. This is meant to express a particular concern related to the advancement of the field from a former co-editor of *Acta Crystallographica* to a current co-editor of *ACA RefleXions*. In particular, I have strong reservations about implicitly aligning our field with recent extensive legal - political efforts to advance the cause of science reported on page 20 of the spring issue. We should be careful for what we wish since the advances we may attain by legal - political means can potentially be marshaled to silence academic freedom so central to scientific inquiry. As we have long known, the very nature of the scientific process must encourage and allow for testing hypotheses which lie outside accepted theories, paradigms and even laws. The courts are not the venue in which scientific understanding and knowledge can be established.

My concern is that the comments on page 20, without some counterbalancing view, seem to open the door for such an implicit alignment. The book referenced on these recent legal endeavors, *Monkey Girl: Evolution, Education, Religion, and the Battle for America's Soul* by Edward Humes, implies that no controversy exists concerning Darwinian evolution on scientific grounds. Unfortunately, this does not acknowledge the groundbreaking work over the past twenty years of the most eminent palaeontologist in China, Jun-Yuan Chen. He is a Chinese styled evolutionist–who challenges Darwinian versions of the same. Enclosed is a copy of a 2003 report summarizing the anti-Darwinian evidence provided by the extensive fossils discovered in 1984 in Yunnan Province

of South China. Although reported by a scientific journalist with ID (Intelligent Design) affiliation, the facts reported can be confirmed by a literature search of the many publications by Chen and his colleagues during the past twenty years. In 1999, the scientists who had unearthed these fossils hosted a conference attended by sixty biologists and paleontologists from around the world to examine the fossils and to listen to both anti- and pro- Darwinian views. To the Chinese scientists the fossil evidence clearly disputes Darwinian versions of evolution. Incidently, Michael Denton, a New Zealand geneticist, attended the Chinese fossil conference. His picture is on page 23 of this article. He is the author of the book, *Evolution, A Theory in Crisis*. This book provides a good summary of the evidence challenging Darwinian evolution which had arisen from within various scientific fields prior to 1985 when it was first published.

In closing, I would like to commend you for your outreach efforts to educate the public on crystallography, to attract young people to our field and to provide ACA members relevant information–of which the Intelligent Design News column is but one aspect. In the future, I trust that the column will include various scientific viewpoints which are emerging in the debate on this vital issue in which crystallographers such as I have great interest and to which crystallography may yet make important contributions.

With best wishes for you personally and for our field,

Lyle H. Jensen

Editor's note: Lyle enclosed with his letter an article by Fred Heeren: Evolution, Chinese Style (Cosmic Pursuit, summer, 2003), in which Jun-Yuan Chen's work is described. If you would like to obtain a pdf or a hardcopy of this article please email conniechidester@earthlink.net. The complete reference for Michael Denton's book is ISBN: 091756152X, paperback, Adler & Adler, 1986, 368 pp. In later communication Lyle also recommended Genetic Entropy & the Mystery of the Genome by John C. Sanford, ISBN: 1599190028, paperback, Ivan Press, 2005, 224 pp.

The recent ACA meeting in Salt Lake City was typical of recent annual meetings. The program was one of the best in several years. Yet, the overall impression of the meeting was not one of stimulation. As one prominent crystallographer commented the meeting lacked energy. There was no sense of excitement but rather of conducting some ritual.

There is no question that organizing and running the yearly meeting is the most important function of the ACA. These events provide opportunities beyond the program to visit with old friends, exchange technical information and gossip, and interact with a wide array of vendors. Ten years ago one left an ACA meeting with a sense of invigoration that has vanished.

Clearly, this change in the meeting's atmosphere is not because of a lack of effort. The Council and meeting organizers work long hours to make these meetings possible. However, there are many aspects that need to be evaluated with regards to the current situation.

1. Is the current ACA structure of twelve SIG's and three Standing Committees the best way of organizing the sessions?
2. Are there too many sessions? Is it really important to have two or three sessions occurring while the award recipients give their presentations?
3. Can topics be found that will bring small molecule crystallographers, material science crystallographers, macromolecular crystallographers, providers of structural results and users of structural results into a session? Right now the meeting is like four or more meetings all competing for attendees. Interestingly each group believes that the others are the problem.
4. Does it make sense to have the relatively small ACA meeting in cavernous convention centers? Should the facility needs be driven by the vendors exhibit?
5. Does it make sense to have the meetings at resorts and other tourist destinations? Do we need to bribe our members so they will attend?
6. Is the ever increasing cost of the ACA meetings providing good value to the membership and attendees?

All of the above and more need to be considered by both the Council and the membership at large. It may be impossible to generate the excitement of the 1990's at today's meetings. After all that was a time when there were huge changes occurring in crystallographic instrumentation and methods. However, to continue the trend of lifeless meetings will only lead to lower attendance and increased dissatisfaction. It is important that our members should want to attend the annual meeting for the education and renewal it provides them and not simply out of a sense of duty.

Phillip Fanwick and Jeanette Krause

Radu Custelcean Will Receive 2008 Etter Award

The 2008 **Margaret C. Etter Early Career-Award** will be presented to **Radu Custelcean**, Research Staff Member, Oak Ridge National Laboratory, next spring. He will give the keynote lecture at a symposium organized in his honor at the ACA Annual Meeting in Knoxville, TN. Radu has been praised "*for his creative research in crystal engineering of novel and functional metal organic framework structures for selective ion binding*." Because the announcement was so close to the publication deadline, his background and accomplishments will be more properly described in the winter issue of *ACA RefleXions*.

ACA Climate Neutral

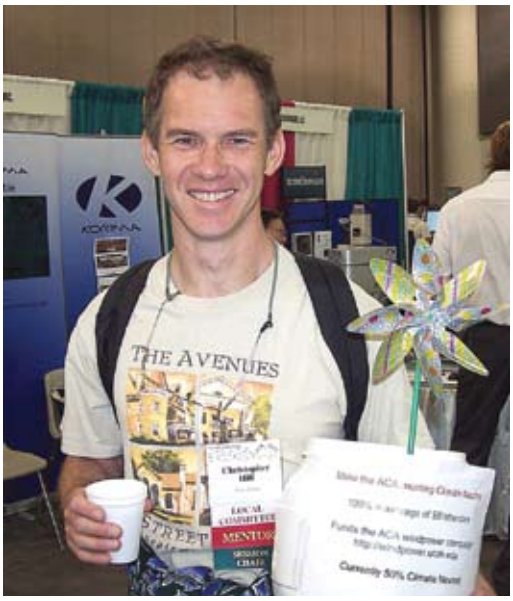

Photo courtesy of Marvin Hackert

As outlined in an editorial in the previous issue of *ACA RefleXions,* we aimed to make the ACA Salt Lake City meeting climate neutral. The concept was to raise funds for a wind energy program that will fund construction of new wind turbines that will supply electricity to the grid and, thanks to the 1978 energy act, thereby displace the use of coal-generated electricity and prevent the release of CO_2 (and mercury). We estimated that if, on average, every individual attending the conference (attendees + exhibitors) donated $5 to the wind energy program, then the CO_2 not released from burning coal would equal the amount of CO_2 emitted from people flying to the conference, staying in hotels, and our share of the conference center.

Thanks to donations from the signers of the previous editorial and donations collected at the meeting, the conference is currently 85% climate neutral. Progress toward and hopefully beyond the 100% goal can be tracked on the web site ***http://windpower.utah.edu***. The program we are using is, we believe, the most cost effective mechanism in the country for individuals to support renewable energy. The campaign will therefore remain open for further donations, which can be made on-line via the web site or by mail-in check, and are tax-deductible. In addition to emissions associated with the conference, this is an effective mechanism to offset emissions associated with other activities at work or home, and also provides the appeal of a campaign-oriented approach for the crystallographic community. For reference, a typical US household's annual electricity use would be offset by a donation of $30/yr, a university worker/faculty/postdoc/student's work electricity ($30/yr), typical US household electricity, heating, and driving ($90/yr), typical US domestic round-trip air-travel ($3-$5) and, at a rough estimate, 24 hours on a synchrotron beamline station ($10).

Our hope is that the campaign will eventually reach or exceed the 100% mark for 2007, and can encourage future meetings by the ACA, IUCr, and other scientific organizations to take similar simple measures to be climate neutral. Similar campaigns are in place for university departments, colleges, and other groups. For example, the University of Utah Department of Biochemistry funded wind energy equal to 154% of its actual use in the 2006/7 academic year. Some other institutions offer similar programs, and if yours does not, we can easily run a campaign on your behalf through the U of U wind energy program. Please send any questions/comments to ***chris@biochem.utah.edu***.

Chris Hill

2007 Spriggs Award to Winnie Wong-Ng

Winnie Wong-Ng, Materials Science and Engineering Laboratory, NIST, along with four of her colleagues, has been selected by the American Ceramic Society to receive the prestigious **Richard and Patricia Spriggs Phase Equilibria Award** in recognition of their paper "Subsolidus phase relationships of the $BaO\text{-}R_2O_3\text{-}CuO_z$ (R=Eu, Dy, and Ho) systems under carbonate-free conditions at T = 810 °C and p_{O2} = 100 Pa," *Physica C*, **439**(2) 93-100 (2006). The authors: Winnie Wong-Ng, Zhi Yang, Lawrence P. Cook, Julia Frank and Mario Loung, are cited for "the most valuable contribution to phase stability relationships in ceramic-based systems" in any professional publication world-wide during the calendar year prior to the selection. This paper is directed towards the processing of practical high-temperature superconductor wires for coated conductor research and development. Winnie Wong-Ng's main research areas in recent years at NIST have been crystallography, crystal chemistry, and phase equilibria of technologically important high-temperature materials, in both bulk and film forms.

Correction:

The editors regret that in the winter, 2006 ACA RefleXions, page 33: the Golden Honor Roll of donations to the ACA Award Funds listed "Carol Chandross in memory of Charles Chandross" His correct name is Ronald J. Chandross.

Reminder: Please VOTE!

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

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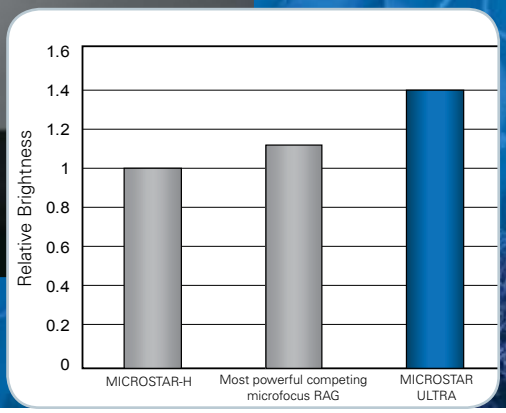
R&D 100 Award Winner



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U.S. Physics Team Wins at International Physics Olympiad

From left: Judy Flippen-Anderson, Andy Lucas, Philip Streich, Haofei Wei. Photo courtesy of the AAPT.

The AIP and the American Association of Physics Teachers (AAPT), both located in College Park, sponsored a ten-day training camp for twenty-four students at the nearby University of Maryland, where the students conducted lab experiments, took exams, and heard presentations from prominent scientists. They also met personally in Washington DC with their Senators and Representatives in the US Congress. The students are part of the International Physics Olympiad, which this year was held July 13-22 at the prestigious Isfahan University of Technology in Isfahan, Iran. The Olympiad is a nine-day international competition among pre-university students from more than 80 nations. The U.S. Physics Olympiad Program was started in 1986 by AAPT to promote and demonstrate academic excellence. The official website of the International Physics Olympiad, hosted by the Iranian team, is **www.ipho2007.ir**

The ACA is also a sponsor of the US Physics team and this year the ACA submitted a series of questions to be included in the preliminary tests, taken by the students all over the country, used to select the 24 students to attend the training camp. The prize for answering the questions correctly was a certificate and a one year membership in the ACA. Eight students answered the questions correctly. Three of them (Andy Lucas, Philip Streich and Haofei Wei) made it to the training camp and Haofei Wei was one of the five students selected to go to the International Olympiad. **Judy Flippen-Anderson** presented the awards to Andy, Philip and Haofei at a reception on June 1st that marked the end of the training camp.

All five of the students selected for the US International Team came home with gold and silver medals: Gold Medalists were **Jason Larue**, Miami, FL; and **Haofei Wei**, Oklahoma City. Silver Medals were won by **Kenan Diab,** Gates Ohio; **Rui Hu**, Wilmington, DE and **Jenny Kwan**, San Marcos, CA "We're proud of our team members and so glad they had the chance to participate in this once-in-a-lifetime experience," said Toufic Hakim, executive director of the AAPT. "We are certainly cognizant of our challenges to attract and prepare physics students to sustain our leadership in the science, but these students do give us hope." Bios of the students are at **www.aapt.org/olympiad2007/team.cfm**; the team websitte is **www.aapt.org/olympiad2007/**.

New! ACA RefleXions Staff Photographer

Peter Müller, Principle Research Scientist, Chemistry Dept., & Director, X-Ray Diffraction Facility, MIT, is a welcome addition to the *ACA RefleXions* staff. The Co-Editors also take photos, and some of them appear in this issue, but Peter's are the ones of professional quality. Look for PM on the photo if the attribution "*Photo by*" is missing.

Photograph by Claire Gallou-Müller, Boston 2005.

Deadline Imminent for NIH EUREKA Awards!

The NIH announces a new program to fund exceptionally innovative research that, if successful, will have an unusually high impact. The program, called EUREKA (Exceptional, Unconventional Research Enabling Knowledge Acceleration), targets investigators who are testing novel, unconventional hypotheses or are pursuing major methodological or technical challenges. The potential impact of the proposed research must be substantial in terms of both the size of the scientific community affected and the magnitude of its impact on the community. **The application receipt date for the EUREKA program is October 24, 2007.** To view the full funding opportunity announcement, see **http://grants1.nih.gov/grants/guide/rfa-files/RFA-GM-08-002.html**.

Travel Bursaries From Rigaku

Rigaku Americas Corporation is pleased to announce the availability of five awards of $500 each to post-doctoral research fellows to help with the costs of travel to upcoming summer meetings such as the ACA meeting in Knoxville, Tennessee (May 31-June 5), the IUCr meeting in Osaka, Japan (August 23-31), and/or another upcoming meeting. One can apply for the award through a simple web form on the Rigaku website: **www.rigaku.com/protein/postdoc.html,** but you must do so before the May 4th, 2008, deadline. The 5 awards will go to the "post-doctoral fellows who provide the most compelling explanation as to how they intend to pursue a career in structural biology."

Jim Pflugrath

SLC Convention Center, Photo by Peter Müller.


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Highlights of Summer ACA Meeting

From left: Alan Pinkerton, Bill Duax, Lisa Keefe, Marvin Hackert, Bernie Santasiero, S.N.Rao, Marcia Colquhoun, Lee Groat.

The ACA Council met just prior to the annual ACA meeting in Salt Lake City, Utah (to conduct business), and frequently during the meeting (the annual business meeting, open to all members, and meetings with the committees whose activities are so vital to the organization). The standing committees and SIG chairs reported on their activities for the last year and presented their plans for the upcoming year. Approximately 50 members attended this summer's business meeting; the minutes are posted on the ACA web site. Key topics that were discussed are summarized here.

Call for Guest Editors for ACA RefleXions: ACA members are invited to contribute to *ACA RefleXions* by being a guest editor for a section of the spring or summer issue. Responsibilities as guest editor include selecting a topic on which several pages of the issue would focus, writing a feature article(s) on the topic, and/or coordinating articles solicited from others on the featured topic. Possible topics are research disciplines, education, technology, user facilities, or methodology. Other topics relevant to crystallography might also be approved. ACA members interested in being a guest editor should contact the editors of *ACA RefleXions*. Council strongly encourages ACA members to take this opportunity to participate in ACA and promote crystallography in their area of interest.

ACA Fellows: Last year, council was presented with the proposal of creating ***Crystallographic Fellows of the ACA*** as a way to recognize outstanding scientific contributions and to serve the crystallographic community. This proposal was presented to the ACA membership at the 2006 business meeting. Following discussions during which council was encouraged to further explore the concept, a motion was made to establish a committee to create a first draft of guidelines. Following through on that motion, a committee was formed and guidelines were drafted and presented at the 2007 business meeting. At this business meeting, the concept of Crystallographic Fellows was discussed extensively, with very mixed views both in favor and against the idea. Council seeks your views on this concept. Please email any council member or ACA headquarters or the RefleXions editors.

Meeting Abstract Book vs. CD: Council is considering transitioning to a CD distribution of meeting abstracts. This move presents several advantages, including lower costs, later deadlines for abstract submission, fewer restrictions on abstract length, and easier archiving. The CDs would be distributed at the meeting while the full abstracts will be available for download from the ACA web site in advance of the meeting. Meeting attendees will still receive in hard copy the meeting program, which will include titles and presenters.

2008 ACA Meeting in Knoxville, TN: The 2008 Annual ACA meeting will be held this spring, May 31 – June 5, in Knoxville, Tennessee. The proximity of Knoxville to Oak Ridge provides meeting attendees the opportunity to visit the newly constructed Spallation Neutron Source (SNS) at Oak Ridge National Laboratory. At this meeting, the Patterson Award will be presented to B.C. Wang. Council looks forward to meeting everyone in Knoxville.

Lisa Keefe, Secretary

TRAVEL FELLOWSHIPS for Osaka IUCr Meeting, 23-31 August 2008

The U.S. National Committee for Crystallography, in cooperation with the ACA, will provide partial support for travel to the International Union of Crystallography Meeting in Osaka, Japan. To be eligible, applicants must be graduate students, post-doctoral fellows, or untenured faculty members in any of the Crystallographic, Diffraction, and Imaging Sciences affiliated with the IUCr. Undergraduate students will be considered in exceptional cases. Applicants must be training at a U.S. institution. Fellows are expected to submit a short report in return for their support after the meeting.

An application should include the following:

(1) Cover page indicating name, address, telephone number, fax, e-mail address, name and address of mentor;

(2) A current Curriculum Vita of the applicant;

(3) Abstract including title and authors, with applicant as presenter, submitted for presentation at the 2008 IUCr meeting;

(4) A paragraph by the applicant describing where they are in their career and why they want to attend the Osaka meeting;

(5) A letter of recommendation from their mentor detailing the group's travel funding and explaining why funds from the USNCCr are needed for the student.

Deadline: 1 March 2008

Send applications to:
Cora Lind
Dept. of Chemistry, MS 602
The University of Toledo
Toledo, OH 43606
(419) 530-1505
FAX: (419) 530-4033
cora.lind@utoledo.edu

The Trueblood Award to Angelo Gavezzotti

The **2007 Kenneth N. Trueblood Award** was presented by ACA President Alan Pinkerton to **Angelo Gavezzotti**, Professor, Dipartimento di Chimica Strutturale e Stereochimica Inorganica, U. Milano at a symposium organized in his honor at the ACA meeting in Salt Lake City. The Trueblood award was created to recognize exceptional achievement in computational or chemical crystallography. Angelo developed, with G. Filippini, the UNI force field. He was also cited for authoring several highly innovative, widely used and successful crystallographic computer programs and for deeply influencing the way we think about molecular packing in crystals. See page 24 for the report on the Trueblood Symposium.

photo by P. Müller

2007 Fankuchen Award to Frank Herbstein

ACA President Alan Pinkerton presented the **2007 Fankuchen Memorial Award** to **Frank Herbstein**, Professor, Dept. of Chemistry, Technion-Israel Inst. of Technology, Haifa, at the symposium organized in his honor. The Fankuchen Award is given to recognize contributions to crystallographic research by one who is known to be an effective teacher of crystallography. Frank was cited for his lifetime achievements in research, teaching and scholarship, and in particular for his recent two-volume encyclopedic work on *Crystalline Molecular Complexes and Compounds* (an IUCr Monograph). See page 25 for the report on the Fankuchen Symposium at the Salt Lake City ACA Meeting.

photo by P. Müller

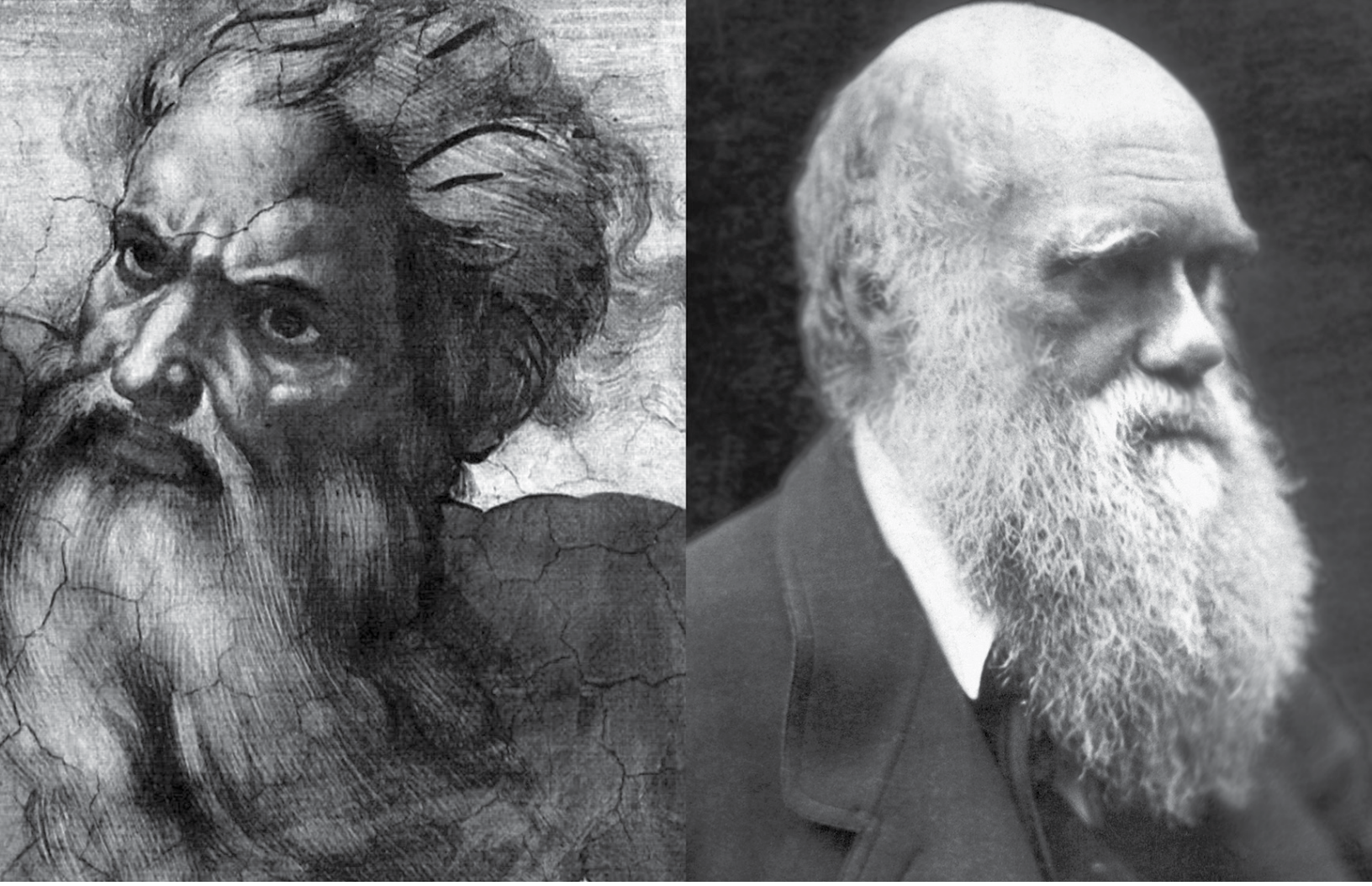
Cora Lind Receives the Etter Award

The **2007 Margaret C. Etter Early Career Award** was presented to **Cora Lind** by ACA President Alan Pinkerton at a special symposium organized in her honor at the Salt Lake City ACA Meeting (see report on the Etter Award Symposium, page 26). Cora joined the U. of Toledo faculty as an Assistant Professor in 2003. Her research program, already thriving and productive, is described on her web site **www.chem.utoledo.edu/FAC_INFO/Lind/SOURCE>htm.** As an educator, Cora has gained the respect of her colleagues for her enthusiasm and professionalism. She revised the curriculum of the graduate x-ray crystallography course, that had previously emphasized small molecule studies, to include the theory and application of several additional methods such as powder diffraction and Rietveld analysis. As the resident powder crystallographer, she manages a facility which includes a new powder diffractometer obtained through her efforts.

Photo of a Salt Lake City Church by Cora Lind.

Alert: Free Generator!

We would like to offer a sealed tube generator free of charge to anyone prepared to pay (up-front) the shipping costs from our laboratory to theirs. The generator has been very little used (as we bought a rotating-anode generator soon after purchase) and is a Rigaku DXG2 2kW (type CN4006A2). It is suitable for small molecule crystallography or for use with strongly diffracting macromolecular crystals. Cabinet size 43.5"(W) x 35.5"(D) x 35.5"(H), weight 350lbs (160 kgs). Please contact Marty Rajaratnam, Randall Division of Cell and Molecular Biophysics, King's College London, r.rajaratnam@kcl.ac.uk if you are interested in acquiring this generator.



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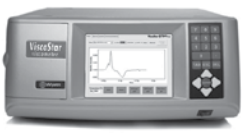

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Poster Prizes at the 2007 ACA Meeting in Salt Lake City

Judging for the 2007 poster competition was organized by John Rose, U. Georgia.

L. to r.: Rebecca Hoeft, Misty Balcewich, Alaji Bah, Ernest Asani, Christopher Jurgenson, Magdalena Korczynska. Photo by Peter Müller.

2007 Pauling Prizes

The **Pauling Prize** is awarded to the best student posters presented at the ACA annual meeting. Up to 5 Pauling prizes may be awarded. In addition a **Canadian Pauling Prize** is awarded for the best student poster from a Canadian institution. The Pauling Prize Committee: **Charles Carter, Ed Collins, Tom Hurley, John Sack, B.C. Wang**, and **Ron Viola**, selected the following students for this year's prizes:

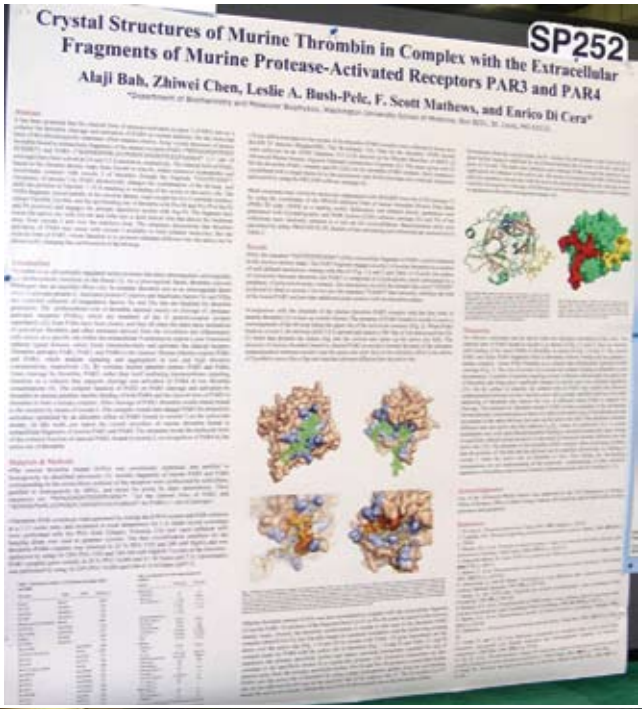
Ernest Asani, New Mexcio Highlands U. for **SP199**: ***Crystal Structure of [1,2,3-$^{13}C_3$]-1-Phenylsulfiny-3-Benzyloxyacetone and Related Labeled Compounds for Isotopically Labeled Materials***;

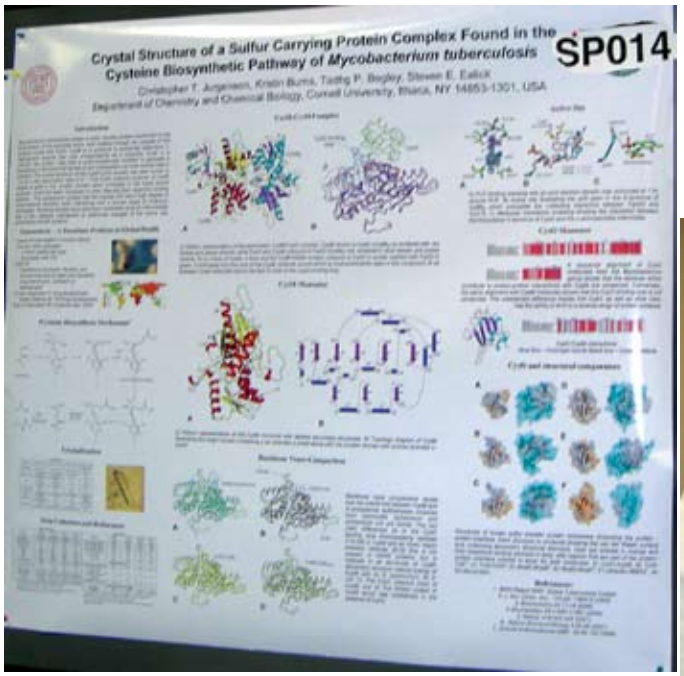
Alaji Bah, Washington U. School of Medicine for **SP252**: ***Crystal Structures of Murine Thrombin in Complex with the Extracellular Fragments of Murine PAR3 and PAR4;***

Misty Balcewich, U. Manitoba for **SP104**: ***Structural Analysis of the Vibrio Chloerae ß-Glucosaminidase NagZ in Complex with PUGNac;***

Rebecca Hoeft, U. Minnesota for **SP138**: ***A Study of Differing Oligomeric Forms of Protocatechuate 3,4-Dioxygenase;***

Christopher Jurgenson, Cornell, for **SP014**: ***Crystal Structure of a Sulfur Carrying Protein Complex Found in the Cysteine Biosynthetic Pathway of Mycobacterium tuberculosis.***

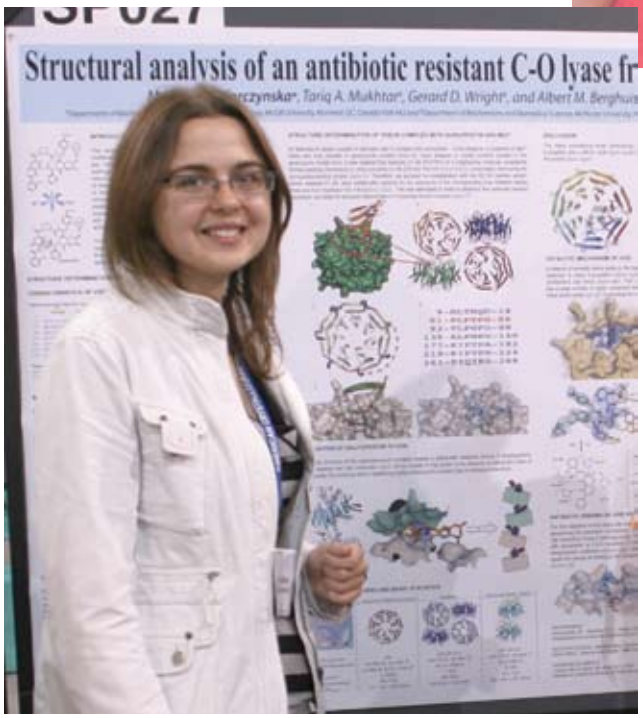




At right: Ernest Asani with his poster. Photo by Victor Young.

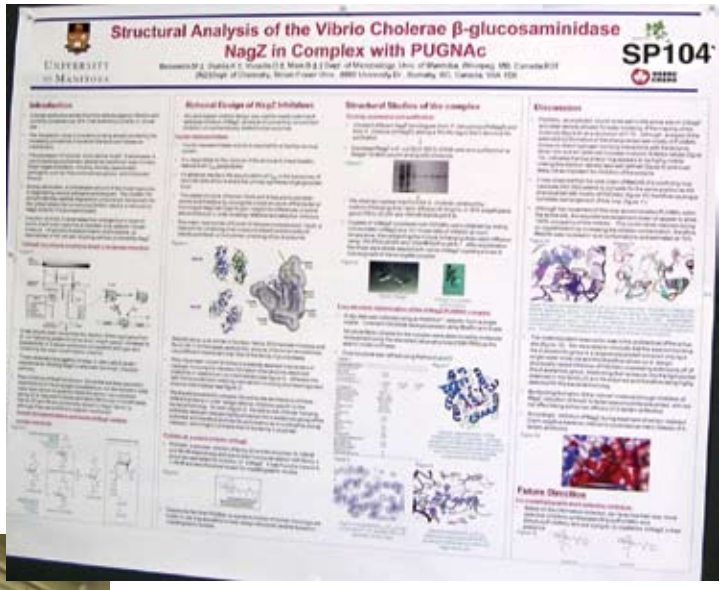
Pauling Poster Prizes, cont'd. The Pauling Prize Committee also selected the following as the best student poster form a Canadian Institution: **Magdalena Korczynska**, McGill U., for **SP027**: ***Structural Analysis of an Antibiotic Resistant C-O Lyase from Staphylococcus aureus.*** She previously won the ACA-IUCr Poster Prize for best poster from North America. Magdalena is shown with her poster, below.

(Photo by Cora Lind).



Rebecca Hoeft, left, with U. Minnesota colleagues Medora Huseby and Carrie Wilmot. Rebecca's poster, SP038 is not shown.

Below, Misty Balcewich's poster, SP104.



Oxford Cryosystems Prize

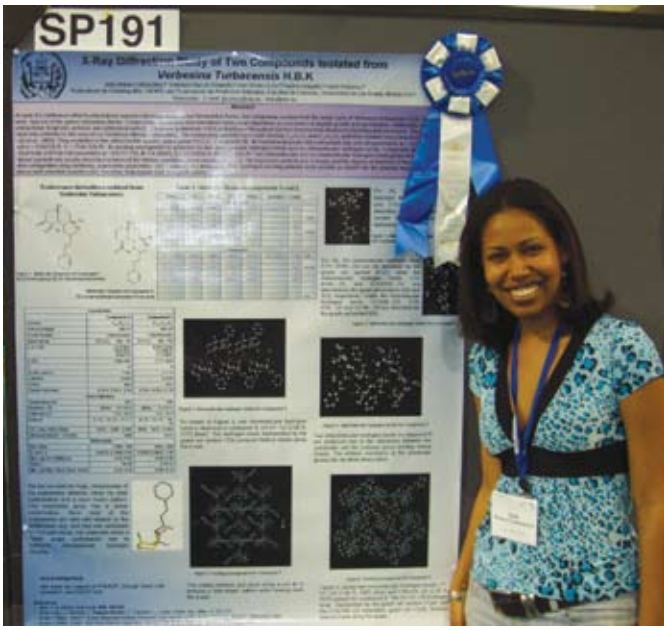
The **Oxford Cryosystems Prize** is awarded to the best poster presented at the ACA annual meeting in the area of low temperature crystallography. The Oxford Cryosystems Prize Committee, **Leif Hanson, Håkon Hope, David Rodgers** and **Edward Snell** selected **Frank Fronczek**, Louisiana State U. for his poster **SP201**: ***Twin Upgrades by Temperature Control***.

At left, Frank Fronczek demonstrating his poster. Photo by Victor Young.

Journal of Chemical Crystallography Prize

The **JCC Prize** is awarded to the best student poster presented at the ACA annual meeting in the areas of chemical crystallography or small molecule structure determination or analysis. For the 2007 prize, the JCC Prize Committee: **Jim Britten, Judith Gallucci, M. Gary Newton** and **Victor Young** selected **Julia Bruno Colmenarez**, Universidad de Los Andes, Venezuela, for her poster **SP191**: ***X-Ray Diffraction Study of Two Compounds Isolated from Verbesina turbacensis H.B.K***. Julia is currently completing her undergraduate studies.

The photo at right showing Julia with her poster is by Victor Young.

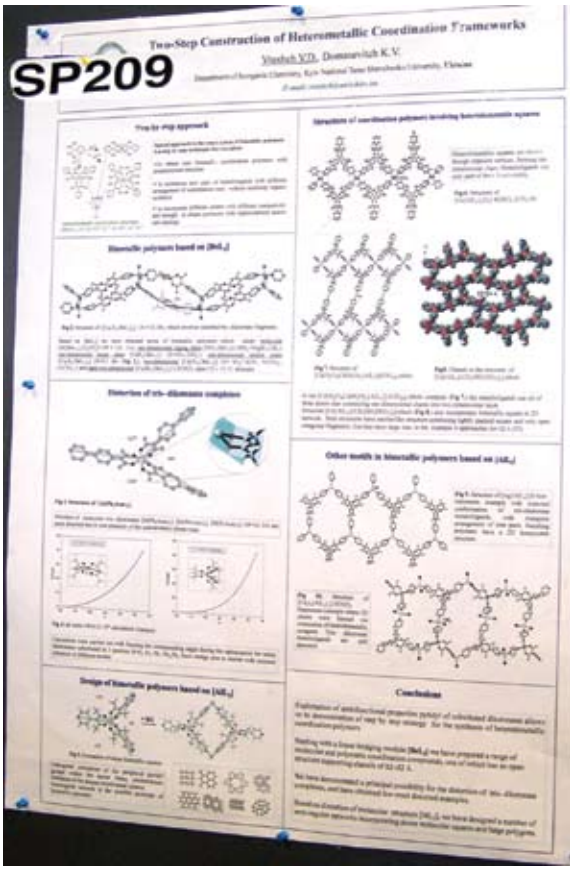


Hasan Demirci and his poster, below.
At left, Hasan with Winnie Wong-Ng.

RSCB Protein Data Bank Prize

The **RSCB Protein Data Bank Prize** is awarded to the best student poster presented at the ACA annual meeting in the area of macromolecular crystallography. For the 2007 Prize, the RSCB Protein Data Bank Prize Committee: **Mitch Guss, Peter Horanyi, Thomas Koetzel, James Phillips, Bernard Santarsiero** and **Timothy Umland**, selected **Hasan Demirci**, Brown U. for his poster **SP003**: ***Structure Based Protein Engineering of Ribosomal Protein Trimethyltransferase.*** His presentation featured a nice slide show of the reaction pathway.

The Pioneer Day Parade in Salt Lake City. The photo on the right is by Cora Lind.



IUCr Poster Prize

The **IUCr Poster Prize** is awarded to the poster presented at the ACA annual meeting with the best look, content and presentation. For the 2007 award, the IUCr Prize Committee, **Charles Carter, Ed Collins, Tom Hurley, John Sack, B.C. Wang**, and **Ron Viola**, selected **Volodymyr Vreshch**, Kyiv National Taras Shevchenko U., Ukraine, for his poster **SP209**: ***Two-Step Construction of Heterometallic Coordination Frameworks***.

The photo of Volodymyr Vreshch at right is by Peter Müller.

Volodymyr's poster is at left.

At right, at the ACA Awards Banquet: Katherine Kantardjieff presenting the AIP URS Prize to Leslie Williams. Photo by Cora Lind.

AIP Undergraduate Research Prizes

All posters submitted to the **Undergraduate Research Showcase, SP.01**, organized by **Katherine Kantardjieff**, were upgraded to talks. Students who gave oral presentations at this symposium were considered for two prizes sponsored by the American Institute of Physics. To be eligible for these awards the students had to describe research that had a significant crystallographic component and that demonstrated a command of the science. In addition they must have done the majority of the work presented. The judges for this year's prizes were **Christopher Cahill, William Furey, Katherine Kantardjieff, Joseph Ng** and **Victor Young**. The winning talks were presented by **Leslie Williams**, U. British Columbia, who characterized the catalytic boost provided by an alternative anion in human pancreatic α-amylase, an important drug target in the treatments of diabetes and obesity, and **Brett Hanson**, Rochester Inst. Tech., who discussed his work with the open source molecular modeling tool, PyMOL, to create a user friendly graphical user interface called ProMOL, which simplifies a number of complex PyMOL functions. See also the report on this symposium, p.27.

Leslie Williams and Brett Hanson with their awards. Photo by Peter Müller.

Durward William John Cruickshank (1924-2007)

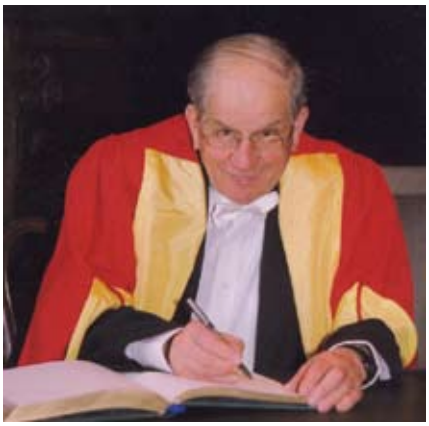
Crystallography today in general and the IUCr in particular owes much to Professor Durward Cruickshank FRS, an eminent crystallographer and structural chemist of high mathematical ability. He died of cancer, peacefully, July 13th, 2007 in his home village of Alderley Edge near Manchester. He 'retired' as Professor of Theoretical Chemistry at the University of Manchester Institute of Science and Technology (UMIST) in 1983 but continued to collaborate very actively until his death, with his last paper in *Acta Cryst*. (2007). **D63**, 906-922 still in press.

Durward Cruickshank transformed the precision of molecular structure determination in 3-dimensions by x-ray diffraction with research publications that span 60 years and that influenced at least 450,000 chemical structures (the number currently held in the Cambridge Structure Database alone). Research on proteins took his attention throughout his last decade and the Cruickshank Diffraction Precision Index (DPI) indicator of the precision of a protein structure is now added regularly to many of the protein 3D structures deposited in the Protein Data Bank. His first paper in *Acta Cryst*.: "The Accuracy of Electron-Density Maps in X-Ray Structure Analysis" was published with Gordon Cox in Volume 1, pages 92-93. His final paper was on the determination of protonation states in proteins, in which his early studies on oxalic acid dihydrate and his interests in gas phase electron diffraction came to the fore. He published over 80 papers in *Acta Cryst*. from 1948 onwards on many topics in crystal structure refinement.

Cruickshank was an early pioneer in the use of digital computers. He would travel from Leeds to Manchester, where Ferranti Ltd. commercialized the first stored-program digital computer, for round-the-clock runs of crystallographic computations. He attended the 1950 Cambridge Summer School on Programme Design for Automatic Digital Computing Machines, which was amongst the world's first summer schools on electronic computing and which introduced him to the principles of computer programming, machine order codes and binary arithmetic.

Durward was born in London on 7th March 1924 and educated at St. Lawrence College, Ramsgate. His career started at Loughborough College, now Loughborough University, as an engineering student. He won an external degree from London University in 1944, then worked until 1946 for the Admiralty on Naval Operations Research. He subsequently studied mathematics at Cambridge, "learning at the feet of Bondi, Hoyle, Boys and Dirac" as he would put it, and was awarded successively his BA (1949), MA (1954) and finally DSc (1961). His entry into the world of crystal structures began in 1946 when he joined E. G. Cox's (later Sir Gordon Cox) chemical crystallography group at Leeds University.

His first academic appointment was as Lecturer in Mathematical Chemistry at the University of Leeds in September 1950. He became Joseph Black Professor of Chemistry at Glasgow University from 1962 to 1967, then was invited to UMIST in 1967 for appointment as Professor of Theoretical Chemistry. Upon retirement in 1983, he became Emeritus Professor at UMIST and, latterly, at The University of Manchester. He was Deputy Principal of UMIST, 1971-1972, made a Companion of UMIST in 1992, and awarded an Honorary Degree by UMIST in 2004. He also received an Honorary DSc from Glasgow University (photo at left) which named their Diffraction Laboratories after him.



His major contributions were formally recognized by the Royal Society, which elected him a Fellow in 1979, and also by other prizes and awards. Notably, he won the Chemical Society (now Royal Society of Chemistry) Award for Structural Chemistry in 1978 and the first Dorothy Hodgkin Prize of the British Crystallographic Association (BCA) in 1991. He delivered the prestigious Bragg Lecture at Leeds University during the annual BCA Conference of 1997, and to the public at The Royal Institution in London, where both Braggs, father and son, had worked. The Braggs are still the only father and son to be jointly awarded a Nobel Prize together (in physics, 1915, "for their services in the analysis of crystal structure by means of x-rays").

Photo courtesy of the Royal Society.

Cruickshank devoted much effort to the IUCr. He was elected IUCr Treasurer in 1966 at the General Assembly and Congress in Moscow for the period 1966 to 1969. The office of Treasurer was combined with that of IUCr General Secretary at the General Assembly and Congress in Stony Brook, N.Y. in 1969 where he was elected to serve in that joint office from 1969 to 1972. Under his guidance, the total financial assets of the IUCr grew steadily in this period to double their value, until his final year when the rising costs of publication and editing and a small erosion of the subscription base resulted in a small loss. These two offices together demanded and received an unusually high level of time and thought. His sage advice was subsequently sought by the IUCr on a variety of occasions. Cruickshank also served as an Editor of the 1992 IUCr memorial volume *P. P. Ewald and his Dynamical Theory of X-ray Diffraction* commemorating Paul Ewald, the founding father of the IUCr. Cruickshank's first contact with the international crystallographic community was at the small Leeds symposium

held in 1948 that attracted many participants from the X-Ray Analysis Group conference held some days previously in London. This led to the formation of the IUCr. (There is a photograph of the event in *Acta Cryst*. (1989). **A45**, 585.

Cruickshank also served the BCA as Vice President 1983 - 1985, was admitted an Honorary Member of the BCA in 2003 and continued to contribute enthusiastically to BCA activities until his death.

Durward Cruickshank was always upbeat, kind and helpful, urbane and gracious. He inspired the love and affection of family and colleagues, was utterly trustworthy and sincere, and could always be turned to for advice. His deep insight into science extended to its history. He liked to emphasize, as his 80th birthday celebration notes show, that there had been relatively few years over which modern science had arisen, *i.e*. (his examples) between Newton's theory of gravitation, Dalton's atomic theory and Watson and Crick's DNA double helix model. Newton, he also noted, was the first person with the mathematical capability of understanding space flight. Looking to future major advances, he highlighted molecular biology and drug discovery, which he judged were still in their infancy. He could also be quite firm. At the BCA's Annual General Meeting in York in 2003, the question of introducing the category of "Fellow of the BCA" arose. Durward spoke successfully against the motion, saying that such a hierarchical membership structure would put the egalitarian nature of crystallography in jeopardy.

In retirement, he renewed his interest in his family tree, visiting the extensive genealogical records archived in Salt Lake City. He was a keen golfer and an enthusiastic member of the Manchester Literary and Philosophical Society. He became interested in the Antarctic and Arctic, visiting both and noting that numerous islands and other features in the Antarctic were named after crystallographers. There are many thousands of topological features in Antarctica for which the Antarctic Place-Names Committee is the responsible British naming authority and which chooses the names of prominent pioneers in techniques that helped to elucidate Antarctic problems, including the structure of ice.

Durward's wife Marjorie predeceased him; he is survived by a son and a daughter and five beloved grandchildren. He will be sadly missed by the whole community.

Sidney C. Abrahams and John R. Helliwell

On the Cover: New Structures at the Salt Lake City ACA Meeting this July

On the right: from **Karl Volz**, U. Illinois Chicago: The structure of IRP1 (4 domains in red, yellow, green and blue) in complex with ferritin IRE-RNA, (left side). Iron regulatory protein 1 (IRP1) binds iron responsive elements (IREs) in messenger RNAs to repress translation or degradation, or can bind an iron-sulfur cluster, to become a cytosolic aconitase enzyme. The unresolved loops are drawn as dotted lines. This 2.8 Å crystal structure of the complex shows an open protein conformation compared with that of cytosolic aconitase. W.E.Walden, A.J.Selezneva, J.Dupuy, A.Volbeda, J.C.Fontecilla-Camps, E.C.Theil, K.Volz, *Science*, **314**, (2006), 1903-1908.

On the left: from **Gerwald Jogl,** Brown U.: a composite image from a coordinate interpolation (morph) between two protein-protein complex structures of the methyltransferase PrmA (colored from red to pink) and the substrate ribosomal protein L11 (colored from dark blue to cyan). The departure of the lysine substrate (moving from the active site to the left) and the arrival of the N-terminal amino group in the active site (from the right) are shown. The bacterial methyltransferase PrmA trimethylates the N-terminal α-amino group and several lysine residues in the N-terminal domain of the ribosomal protein L11.[1] Protein L11 consists of two domains of approximately 70 amino acids: a C-terminal 23S rRNA binding domain and an N-terminal domain that has been shown to contact elongation factors G and Tu.[2,3] This domain also forms part of the binding site for the antibiotic thiostrepton and mutations in the N-terminal domain confer thiostrepton resistance.[1] However, despite the active role of L11 in ribosome function, the function of L11 methylation by PrmA has not been identified because prmA-null mutants remain viable.[4]

We have studied the unusual capability of the PrmA methyltransferase to modify several lysine side chains (and the N-terminal amino group) on the same substrate protein. The structure of PrmA has been determined previously[5] and consists of a larger class I methyltransferase domain and a smaller substrate recognition domain connected by a flexible linker region. We have determined crystal structures for 8 unique conformations of PrmA in a total of 11 unique crystal forms that include 4 unique PrmA-L11 complex conformations.[6] Two complex structures capture Lys39 and the N-terminal amino group of L11 positioned in the active site in a pre-catalytic and post-catlytic state, respectively. Two non-catalytic complex structures were obtained from site-directed mutants of protein L11.

Our results show that the L11 substrate protein is recognized by a ß-sheet docking mechanism between the PrmA substrate recognition domain and the L11 N-terminal domain. The flexible linker between the two PrmA domains allows the enzyme to position the substrate in a large number of conformations relative to the catalytic domain.

1. D.M.Cameron, J.Thompson, S.T.Gregory, P.E.March, A.E.Dahlberg, (2004) *Nucleic Acids Res.* **32**, 3220-3227.
2. B.T.Wimberly, R.Guymon, J.P.McCutcheon, S.W.White, V.Ramakrishnan, (1999) *Cell* **97**, 491-502.
3. R.K.Agrawal, J.Linde, J.Sengupta, K.H.Nierhaus, J.Frank, (2001) *J. Mol. Biol.* **311**, 777-78.
4. D.M.Cameron, S.T.Gregory, J.Thompson, M.J.Suh, P.A.Limbach, A.E.Dahlberg, (2004) *J. Bacteriol.* **186**, 5819-5825.
5. T.Kaminishi, H.Sakai, C.Takemoto-Hori, T.Terada, N.Nakagawa, N.Maoka, S.Kuramitsu, M.Shirouzu, S.Yokoyama, (2003) *Acta Crystallogr D* **59**, 930-932.
6. H.Demirci, S.T.Gregory, A.E.Dahlberg, G.Jogl, (2007) *EMBO J.* **26**, 567-577; also unpublished data.

Editor's note: see the report on the New Structures session, pages 28-29. Also please note that there were many new structures presented at this meeting that were reported in other sessions.

Contributors to This Issue

Sidney Abrahams, Paul Adams, Joel Bernstein, Rick Bott, Carol Brock, Paul Butler, Sue Byram, Branton Campbell, Bryan Chakoumakos, Julian Chen, Vivian Cody, Carl Correll, Radu Custelcean, Thomas Earnest, Larry Falvello, Phillip Fanwick, Richard Gillilan, Israel Goldberg, Eduardo Granado, Lee Groat, Günter Grossmann, Andreas Heine, William Heller, John Helliwell, Chris Hill, Jason Hodges, Peter Horanyi, John Horton, Jacques Huot, Ashfia Huq, Jan Ilavsky, Theodore Jardetsky, Lyle Jensen, Gerwald Jogl, Werner Kaminsky, Katherine Kantardjieff, Lisa Keefe, Jeanette Krause, Paul Langan, Byeongdu Lee, Cora Lind, Kenneth Littrell, Dave Matthews, Ethan Merritt, Peter Müller, Dean Myles, Chris Nielsen, Bruce Noll, Allen Oliver, Jim Pflugrath, Paula Piccoli, Alan Pinkerton, Lionel Porcar, Claudia Rawn, John Rose, Gerd Rosenbaum, Tim Rydel, Jack Sack, Ron Stenkamp, P. Thiyagarajan, Iris Torriani, Yingssu Tsai, Volker Urban, Karl Volz, Bi-Cheng Wang, Manfred Weiss, Thomas Weiss, Richard Welberry, Kraig Wheeler, Winnie Wong-Ng.

Special thanks to Kathy Kantardjieff, Cora Lind, Peter Müller, Marvin Hackert, and Victor Young for supplying photographs taken at the annual meeting. Peter sent so many that he is now ACA RefleXions staff photographer (see p. 7). If credits are not noted as "photo by" they are indicated on the photo with initials of the photographer, e.g. CL for Cora Lind.

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Top row pictures, from left: Tom Koetzle with Cheryl, Ricky, and Ed Stevens; Zheng-Qing Fu talking with Mark Pressprich; Louis Delbaere, Carol Delbaere, Florence Quail, Sue Byram, and Wilson Quail. Next row: Bryan Chakoumakos;* Lisa Keefe and Osnat Herzberg; Leif Hanson and Chick Wilson. Third row: Julia Bruno Colmenarez and Graciela Diaz de Delgado; Yihau Huang, Richard Baxter and Charles Dann. Bottom left Ron Viola and Bi-Cheng Wang; Howard Einspahr and Judy Flippen Anderson.**

** Photo by Peter Müller.*

2007 ACA Meeting - Salt Lake City, UT, July 21st-26th

Highlights of the meeting included presentation of the **Kenneth N. Trueblood Award** to **Angelo Gavezzotti**, the **Isidor Fankuchen Award** to **Frank Herbstein**, and the **Margaret C. Etter Early CareerAward** to **Cora Lind** (see p. 10). Reports on the symposia organized in their honor are on pp 24-26. See also the many poster prizes awarded on pp. 12-15. **Lisa Randall** was presented with the **Elizabeth A. Wood Award** at the Awards Banquet; photos taken at the banquet are on page 30 -31. The ***Transactions* Symposium**, organized by **Branton Campbell** was on ***Diffuse Scattering for the Masses ...,*** see report, pp 22-23.

Program Chair **Jill Trewhella** and the entire Program Committee deserve congratulations for organizing a diverse and scientifically exciting program. The Program Committee and session organizers raised far more money to help sessions bring in speakers than has ever been done before, and this contributed significantly to the success of the meeting. To recognize their efforts and to recognize the major donors for their largesse, a new feature of the meeting, the **President's Reception** was held. Pictures from that reception occupy most of this page. The winter *ACA RefleXions* will carry reports on the workshops, and by the Travel Award winners, as well as photos of the YSSIG Mixer, the Mentor-Mentee Dinner, and various parties and events sponsored by our generous vendors. Seven hundred twenty-five people registered for the meeting; there were 297 talks and 250 posters.

Our indefatigable Local Chairs **Chris Hill** and **Heidi Schubert** are at left below. The picture here is one of the few pictures of Chris where he is not holding the "Climate Neutral" pot; see his article, p. 4. Program Chair **Jill Trewhella** is at right, below, talking with Volker Urban, a Session Chair.

See p. 18 for credits for meeting photos. Unless otherwise noted, the photographs of session speakers were taken by people who managed the AV equipment: U of U graduate students Beth Stadtmueller, Brian Kelly, William Shum, Jason Schalle and Hongbo Pang; by Joe Burg, an undergraduate student, and by Daniel Krauchuk, an MD who happened to be interested.

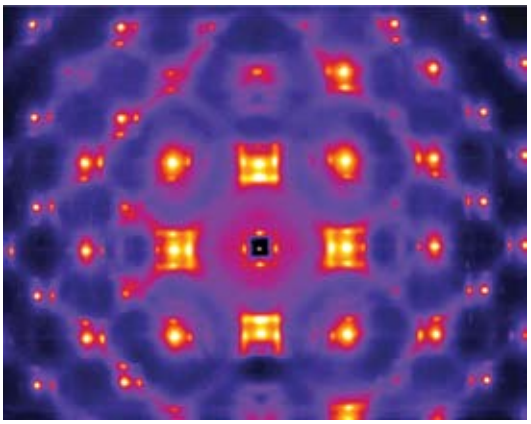
Above, from left: Jim Kaduk, John Horton, Heidi Schubert, Paul Swepson, Patrick Bronson-Doherty, Haruko Hamlin, Peter Horanyi, Judy Flippen-Anderson, Ron Hamlin, Joel Bernstein. Below, from left: ACA President Alan Pinkerton, Branton Campbell, Bob Von Dreele, Cora Lind, Marcia Colquhoun, Bernie Santasiero.

TR.01 Transactions Symposium

The topic of the 2007 *Transactions* symposium was "Diffuse scattering for the masses: the characterization of local structural correlations in molecular, macromolecular and inorganic crystals," which reflects the now common observation of diffuse features in area-detector images from virtually all material classes, and the increasing awareness that local structural features strongly influence many of the useful properties of real crystals. The papers presented at the symposium will be published online via the ACA website, thanks to the efforts of our *Transactions* editor, **Jim Britten**.

From left: Abbas Ourmazd, Lars Meinhold, Andrew Beasley, Richard Welberry, George Phillips, Branton Campbell.

Richard Welberry, Australian National U., demonstrated the use of highly-versatile Monte Carlo simulation methods to analyze and interpret diffuse scattering patterns. By strategically exploring a small number of interaction parameters (e.g. intermolecular spring constants, intramolecular torsion constants, local displacement-displacement correlation coefficients, etc.) one can identify atomistic disorder models that reproduce experimental diffuse scattering features. Specific examples included framework faulting in zeolite catalysts, nanopolar domains in ferroelectric relaxor $Pb(Zn_{1/3}Nb_{1/3})O_3$, and orientational disorder in penta-chloro-nitro-benzene.



From Richard Welberry: stationary crystal (Laue) exposure of the non stoichiometric oxide wüstite, $Fe_{1-x}O$. This single frame of data was recorded on a Mar345 Image Plate detector at beamline 1-ID-C at the APS with a 3 second exposure and 80keV x-rays. The incident beam was directed approximately down the cubic 4-fold axis. A wealth of detailed diffuse scattering is revealed, providing information about the complex defect structure of wüstite. This includes information concerning the nature of the defect clusters, their distribution in the surrounding rock-salt type FeO lattice and the way the latter is locally distorted by the defects. T.R.Welberry, A.G.Christy. Phys. Chem. Minerals, (1997) 24, 24–38.

Branton Campbell, Brigham Young U., reviewed the challenges and prospects of fitting local-structure models against complete volumes of diffuse scattering data, which make it possible to simultaneously interpret all of the salient features of a complicated 3D pattern. Whereas advances in source and detector technology already make this possible in principle, software is the current bottleneck in three key areas: 3D data visualization, quantitative HKL volume reconstruction, and local-structure model optimization. Novel solutions to the reconstruction and optimization problems were demonstrated for current structural problems in microporous framework compounds, magnetoresistive manganites, high-TC cuprates, and relaxor-based piezoelectrics.

George Phillips, U. Wisconsin, described the use of diffuse scattering (also called variational scattering) to discover the elusive details of protein dynamics. By modeling a protein in terms of inter-residue springs (the Gaussian Network Model), he demonstrated that one can perform a normal-mode analysis to extract dynamical information in the form of a covariance matrix. Specific examples that were presented included diffuse scattering from yeast-initiator tRNA and correlated displacements in Calmodulin, as well as a normal-mode analysis of a PDZ domain. The details of the normal-mode approach were further illuminated during the poster session by **Demian Riccardi**, **MP170**.

Donald L. D. Caspar, Florida State U., was unable to attend due to health complications, but offered the following encouragement: "I was very much looking forward to participating in this symposium since variation is the secret of life, and crystallography could contribute to revealing some of these secrets if looking at all the diffraction data from crystals became more fashionable. I hope that this *Transactions* Symposium will alert adventurous crystallographers to look more carefully at variations in crystal structures."

Andrew Beasley, Australian National U., demonstrated the quantitative fit of an inter-molecular force model to a disordered polymorphic organic system. Each step of the fit involved a Monte-Carlo simulation of a large-scale atomistic model, the simulation of the associated diffuse scattering patterns, and a comparison against multiple 2D sections of experimental diffuse scattering data. In addition to the actual polymorphic structure, this promising approach yields the details of the intermolecular forces that crystal engineers may use to predict and control polymorph formation.

Lars Meinhold, Caltech, emphasized that protein function depends on both structure and dynamics. While the average structure is accessible via Bragg scattering, the diffuse scattering reveals dynamics. Lars presented the use of molecular dynamics simulations to determine the macromolecular phonon vibration spectrum and the conformation energy landscape. Calculated displacement patterns and conformational distributions were then validated by simulating diffuse scattering patterns and comparing them against 1D, 2D, and 3D experimental reciprocal space data.

Abbas Ourmazd, U. WI-Milwaukee, proposed a novel solution to the random-orientation problem that affects the prospects of single-macromolecule structure determination at the next generation of x-ray sources (*i.e.* XFELs). Rather

than attempting to coax each molecule into a standard alignment prior to its pulse of x-rays, and averaging the scattering patterns of each molecule probed, one freely allows random orientations and saves the scattering patterns of each molecule separately. A statistical correlation technique (Generative Topographic Mapping) then recovers the orientation of each molecule after the fact. Advantages of this approach include noise robustness and discrimination, thus mitigating the anticipated low photon counts in each diffraction pattern.

L. to r.: Stephan Rosenkranz, Branton Campbell, Ross Angel, Jim Britten, John Konnert, Simon Billinge, Frederick Frey.

Friedrich Frey, Ludwig-Maximilians U., Munich, introduced the foundational concepts of diffuse scattering for newcomers to the field, and illustrated them with practical examples from the complex oxides. These included the description and experimental identification of the average structure, size and strain effects, anisotropic displacement parameters, static displacements, substitutional/chemical short-range order, systems without any long-range order, and domain disorder, as well as descriptions of some common interpretive errors. He concluded by demonstrating that aperiodic crystals are subject to these same types of disorder and also produce intricate diffuse scattering patterns.

Stephan Rosenkranz, Argonne, presented plans for CORELLI, a dedicated single-crystal time-of-flight neutron diffuse-scattering instrument with elastic-energy discrimination to be built at the new Spallation Neutron Source. CORELLI will enable efficient 3D coverage of reciprocal space with high resolution for large samples, and will permit the separation of elastic diffuse scattering from inelastic processes such as thermal diffuse scattering. He explained that by employing a statistical chopper and cross correlation, CORELLI will utilize of up to 50% of the available incident spectrum, and therefore provide a large efficiency gain compared to conventional energy-discrimination methods that have been applied to diffuse scattering.

Simon Billinge, Michigan State U., updated us on the state-of-the-art in powder pair-distribution-function analysis: dedicated neutron PDF instruments, rapid x-ray PDF data collection strategies, open-source PDF analysis software, and a variety of local-structure model classes that can be applied to PDF data. He demonstrated the application of PDF techniques to $Mo_6S_xI_{1-x}$ nanowires, Na-intercalated silica gels, and CdSe nanoparticles, and emphasized that quantitative structural information provides predictive power. In conclusion, Simon showed that PDF analysis, in addition to being an efficient refinement tool for local-structure models, might also be used for nanoparticle structure determination.

Jim Britten, McMaster U., illustrated the application of modern graphic-visualization routines (the Max3D package) to explore volumes of reciprocal space. Max3D loads raw area-detector images obtained during a standard crystallographic data collection, and provides breathtaking birds-eye views of the diffuse-scattering distribution throughout the rendered volume. Jim surprised the audience with a variety of heretofore unseen diffuse-scattering patterns from well-studied materials that were collected on a standard laboratory diffractometer. This new development underscores the importance of collaboration between the physical and computer sciences.

Ross Angel, Virginia Tech., emphasized that his perspective is that of a typical "user" of crystallographic tools who has no special training in diffuse scattering methods, and presented a number of striking diffuse-scattering features that he has encountered on a standard area-detector-equipped lab diffractometer. In many cases a qualitative interpretation of the diffuse features returned a wealth of local-structure information and clues to its chemical/physical origins. In the cases of nepheline and $Fe_{1-x}O$, Ross demonstrated that parametric studies (e.g. pressure and temperature) of diffuse scattering can provide unique insights into the mechanisms of phase transformations and structural instabilities. The diffuse scattering from octakis-octasilicate, and the unusual columnar faulting implicated, was further described by **Carla Slebodnick,** Virginia Tech, in poster **MP169**.

John Konnert, Naval Research Lab., described the analysis of x-ray diffuse scattering from low-dimensional orderings in a liquid-crystal elastomer comprised of two cross-linked molecular components. By mapping out an entire 3D reciprocal-space volume (using a phi-rotation sequence and an area detector), rather than relying solely on a traditional 2D diffraction image, he was able to substantially improve the constraints on physically-reasonable candidate models. A periodic PDF along the applied-stress direction was then used to qualitatively validate a specific structure.

The symposium presentations demonstrated that a variety of specialized tools are already available. However, for many, diffuse scattering will have arrived as a mainstream analytical method only when these tools come packaged with new diffractometers and detectors. Some key components, such as 3D visualization, are likely to become integrated with standard systems over the course of the next year. Standard GUI-driven tools for generating local-structure models and simulating single-crystal diffuse-scattering patterns are currently feasible and could be available within a few years if the crystallographic community maintains it's current level of interest.

Branton Campbell

AW.01 & AW.02 The Trueblood and Fankuchen Award Symposia

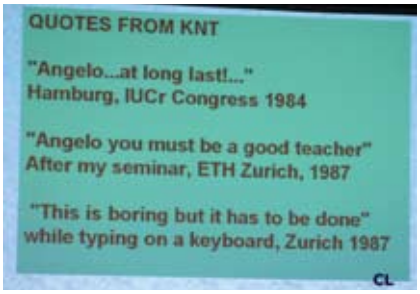
Award ceremonies and symposia are an occasion for celebration, reminiscing, and even a bit of nostalgia. There was a delightful mix of all at the Trueblood Award and Fankuchen Award Symposia.

From left.: Joel Bernstein, Michael McBride, Graeme Day, Angelo Gavezzotti, Peiro Macchi, Jack Dunitz, Carol Brock.

Although there is no formal connection between the two awards, the many common scientific interests and colleagues of this years' awardees, **Angelo Gavezzotti,** U. Milan, **Trueblood Award**, and **Frank Herbstein**, Technion-Israel Institute of Technology, **Fankuchen Award**, suggested combining what is normally two separate half-day functions into a daylong 'festival.' **Carol Brock**, U.Kentucky, and **Joel Bernstein**, Ben-Gurion U.of the Negev, Israel, jointly organized the award ceremonies and symposia.

Beginning with a group photo from Ken Trueblood's retirement symposium in 1989, **Joel Bernstein** recalled some of Ken Trueblood's associates, noting their "contributions to computational and chemical crystallography." (See p. 10 for award citations and ceremony.) Among these collaborations were the application in the 1950s of digital computers to the calculation of electron density (with Dorothy Hodgkin on the Nobel prize winning vitamin B_{12} structure); the first program for least squares refinement (with the late Bob Sparks, then a Ph.D student); one of the first programs, predating *SHELX* and *MULTAN*, for direct methods solution of crystal structures (with Bob Long); the development of rigid body analysis of anisotropic temperature factors (with Verner Shoemaker); and the extraction of vibrational frequencies from those temperature factors (with Jack Dunitz and Emily Maverick).

Following the formal bestowal of the Trueblood Award, **Angelo Gavezzotti** responded by recalling his early days as a Ph.D student at the University of Milan under Massimo Simonetta (who himself had been a postdoc with Linus Pauling at Caltech), and his use of the Trueblood/Long program to solve the one (!) crystal structure that comprised his Ph.D. thesis. He reminisced about his own contacts with Trueblood and described some of his early and recent work and thoughts about the use of computational techniques to characterize and understand crystal structures, the potential for predicting crystal structures, and the possible existence of polymorphs.



The current state-of-the-art in the *ab initio* computational prediction of crystal structures from a molecular structural diagram was described by **Graeme Day**, Cambridge, based on the results of a series of 'blind test' competitions involving more than15 groups around the world. He presented the results of the latest (4th) round, released only a few hours before his lecture. Day's conclusion is that while some progress has been made since these methods were initially developed in the 1950s in the Soviet Union by A.I. Kitaigorodskii, he concurred with Gavezzotti that there is still a great deal to be done before we can predict a crystal structure or the number and structures of polymorphs with any level of confidence.

Jack Dunitz, ETH, Zurich, a long time friend of Ken Trueblood (and Linus Pauling) from their joint days at CalTech, and a frequent collaborator with Gavezzotti, then presented a talk describing the many ways in which fluorine - the "odd man out" by his description - exhibits maverick behavior with respect to most other elements, as revealed by crystallography, spectroscopy and thermodynamics. As he pointed out, "in a molecular assembly fluorine atoms have to go somewhere, and wherever they go you can make a nice story" - which he certainly did. Jack also poignantly remarked on how the crystallographic community, perhaps more than any other discipline in science, is very much a family, and how the community of small molecule crystallographers is a particularly tight-knit branch of that family

Piero Macchi, a current colleague of Gavezzotti in Milan, then described high pressure and low temperature studies on solid-solid phase transitions of a cobalt complex, in which the phase change is accompanied by a significant change in molecular geometry. **Mike McBride** from Yale closed the Trueblood Symposium in his inimitable style with an enticing mix of history and contemporary fundamental questions. He described his recent experiments and accompanying models on the detailed mechanism of the dissolution of crystals of *dl*-serine.

From left: Bill David, Bart Kahr, Gautam Desiraju, Frank Herbstein, Joel Bernstein, Carol Brock. *Photo by Peter Müller.*

The **Isidor Fankuchen Award** was presented to **Frank Herbstein,** (see p. **10**), and Frank responded with a lecture summarizing many of the structural and spectroscopic data on the quintessential π electron acceptor tetracyanoquinodi-methane.

Also mixing the historical, with the contemporary, **Gautam Desiraju** from Hyderabad followed with a provocative talk on the relationship between kinetic and thermodynamic crystal forms, invoking the well-known Curtin-Hammett principle from physical organic chemistry to the competition between kinetics and thermodynamics in the appearance of different crystal forms.

Co-Chair **Carol Brock** returned to the theme of organometallic compounds and described a polymorphic system which, upon cooling from room temperature, reveals the remarkable change in Z' from 1/4→1/2→7→1. The interpretation of the variation in these values, their sequence over the temperature range studied, and the nature of the disorder of those for which Z'≠1 will certainly contribute to the current discussion on the significance of structures of this type in the framework of polymorphic systems. **Bill David**, Rutherford Appleton Lab.,UK, then described the application of synchrotron and neutron powder techniques to the study of three previously (often rather intensely) investigated, but very much still enigmatic systems: adamantine, sulfur (S_8), and pyridine. An apparent isotope effect with pyridine was noted that merits further study, and should stimulate considerable interest.

The final talk of the day was given by **Bart Kahr**, U. Washington. Kahr, a former student of McBride, has a similar lecture style and is a master story teller, mixing history and crystallography and spicing his tales with Woody Allen humor. He related the tale about how Eligio Perucca, a professor of physics at the University of Turin from about 1919-1959, "first observed induced optical activity" – or did he? In addition to the physics and crystallography Kahr sprinkled his lecture with tidbits describing Perucca's reputation among his students, he was thought to be something of a tyrant as an instructor.(This should serve as a warning to other teachers on how long one's reputation can survive.) As it happened, Kahr's tales of Perucca provided the impetus for a rare and truly memorable moment. Unbeknownst to Kahr, the audience was graced by the presence of Davide Viterbo, a longtime faculty member at the same university, who had been a student of physics in one of Perucca's classes. Even before Kahr completed his lecture, Viterbo requested – and was granted - permission to approach the microphone and relate a few personal accounts, confirming Kahr's anecdotal tales of Perucca's classroom tyranny. The question of whether Perucca had first observed induced optical activity is still open to debate, but the lecture, and the atmosphere created by that incident and the day long sharing of academic experiences by the speakers provided a fitting close to a unique day of award symposia honoring two distinguished members of the crystallographic community. It was the stuff memories are made of.

The fact that the awardees, speakers and participants came from all over the world testified to the universality of science in general and of crystallography in particular. Their participation was considerably facilitated by generous financial support from AstraZeneca AB, Hoffmann-LaRoche, Inc., SSCI/Aptuit, the Cambridge Crystallographic Data Centre, and Oxford University Press, which has recently published books authored by the awardees. These contributions to a very special occasion are most gratefully appreciated.

Joel Bernstein and Carol Brock

The London School of Infectious Diseases Isolation Chamber Orchestra ***by Nick D. Kim, U. Waikato, New Zealand. See nearingzero.net/res.html.***

From left: Shao-Liang Zheng, Jamie Wallen, Christophe M.L.VandeVelde, Cora Lind, Andrew Hemmert, Albert Reger, Peter Horanyi, Niket Shah, Benjamin Scott, Tali Lavy.

AW.03 Etter Early Career Award Symposiuim

The session began with the presentation by ACA President Alan Pinkerton of the **Etter Early Career Award** to **Cora Lind**, U.Toledo (see p. 10 for details about the ceremony). Lind's award lecture described her studies using powder diffraction to understand negative thermal expansion materials. Her presentation also demonstrated the flair for mentoring cited by the Etter Award Selection committee.

The other talks in the session were all from student presenters. The first talks focused on small molecules. **Shao-Liang Zheng,** SUNY, Buffalo, began by discussing the uses of supramolecular solids with molecules embedded in them and the E/Z isomerization of these embedded molecules. Another interesting aspect of supramolecular solids was discussed by **Benjamin Scott**, Kansas State U. He explained the role of Bis-pyrazole based ligands in supramolecular synthesis. **Christophe M.L. Vande Velde,** Buffalo State College, showed how charge density measurements are dependent on very precisely determined x-ray structures, emphasizing the care needed to model the contents of the asymmetric unit successfully.

Photo courtesy of Cora Lind

Macromolecular studies were emphasized in the next talks. **Andrew Hemmert,** UNC, enlightened the audience about the use of proteins as vaccines to overcome nerve agent exposure. His work focused on using x-ray structures to aid design of better proteins for this unique purpose. **Niket Shah**, U Toronto, described the structure of Golgi α-mannosidase, an enzyme in the secretion pathway in eukaryotes. **Jamie Wallen**, Wake Forest, described the proposed mechanism of Coenzyme A-disulfide reductase, while amazing the audience with his use of visual aids. **Albert S. Reger**, HWI, showed how the large conformational change observed in his structures of 4-Chlorbenzoate CoA Ligase allows this enzyme to perform two unique half reactions.

The last talk of the session was by **Tali Lavy**, Israel Institute of Technology, who won an **Etter Student Lecture Award**. **Peter Horanyi**, UVA. from the Young Scientist SIG presented the award. Lavy discussed her data on inclusion compounds and the interesting transitions they go through during photochemical reactions as revealed by their structures.

Peter Horanyi

Marilyn Olmstead and Oana Luca in the audience. Photo by Peter Müller.

Photo by Katherine Kantardjieff.

From left: Katherine Kantardjieff, Brett Hanson, Leslie Williams, Stephanie Bettis, Christina Panizales and Gary Brayer.

SP.01: Undergraduate Research Showcase

The second annual **Undergraduate Research Showcase** was extremely well attended for a busy first afternoon of the meeting. Students making oral presentations at this symposium were considered for two prizes sponsored by the American Institute of Physics. This year, the two **AIP Outstanding Oral Presentation Prizes** were awarded to **Leslie Williams** and **Brett Hanson**. See p. 15, the AIP Awards. It may come as no surprise that these two students were also among our Student Travel Award winners!

The first two talks in the symposium were by faculty research mentors, **Katherine Kantardjieff**, Cal State, Fullerton, and **Gary Brayer**, U. British Columbia. Kantardjieff described a very ingenious crystallography course for senior undergraduates in chemistry and biochemistry, which was taught to two groups of students at Cal State Fullerton and Harvey Mudd College using web conferencing and remote diffractometer access cybertools. Brayer then described curriculum materials he has developed as part of his "passing the torch" initiative, which aims to teach crystallography to undergraduate biology majors.

The remaining four presentations were given by undergraduate students. **Stephanie Bettis**, Berry College, presented her research project comparing the tetramethylammonium and sodium salts of 3-nitrophenolate. The structures, determined to examine structure-activity relationships, revealed no statistically significant differences in bond lengths that could be attributed to the presence of different cations. **Leslie Williams**, U. British Columbia, reported her crystallographic studies to characterize the catalytic boost provided by an alternative anion in human pancreatic α-amylase, an important drug target in the treatments of diabetes and obesity. Williams' work reveals that the presence of nitrite alters the position of a catalytic residue D300, and alters the electrostatic potential in the substrate binding pocket. Anion binding may also be a factor in substrate specificity and substrate profiles. **Christina Panizales**, U. Mass., described her efforts to understand, from the structure, the anti-cooperative substrate and metal co-factor binding in inositol monophosphatase from the hyperthermofile *Archeoglobus fulgidus*. X-ray studies are in progress to identify active site residues linked to interfacial contacts in this homodimeric enzyme that may influence conformational changes. Panizales is using crystallographic information to develop fluorescence assays that test the various hypotheses.

Finally, **Brett Hanson**, Rochester Inst. Tech., discussed his work with the open source molecular modeling tool, PyMOL, to create a user friendly graphical user interface called ProMOL, which simplifies a number of complex PyMOL functions. Additional capabilities have been added as well, including electron density map importing and controls, Ramachandran plots, and widgets to measure interatomic distances and create active site profiles for pattern searching against the PDB.

This symposium was extremely well attended on a busy first afternoon of the meeting, and the student presentations were well received by audience and judges alike.

Katherine Kantardjieff

1.01: New Structures

From left: Carl Correll, Laura Guogas, Gerwald Jogl, Carrie Wilmot, Karl Volz, Allen Orville, Da Jia, John Horton, Ya Ha.

What constitutes a "New Structure" in the ever faster paced world of macromolecular structure determination? At best, it is a structure that conveys new information about biology and/or chemistry, and raises more questions than it answers. The structures presented at this year's "New Structure" session met these criteria. Another theme of this session is that one structure is often not enough. To elucidate function it is often necessary to capture views of the macromolecule as it progresses from one intermediate to another along its reaction pathway.

This latter theme was illustrated by **Karl Volz**, U.Ill., Chicago, who presented the structure of a complex of the apo-iron regulatory protein 1 (IRP1) bound to its repressor mRNA and compared it with the structure of IRP1 bound to iron that functions as an aconitase, interconverting citrate and isocitrate. In iron-replete cells, IRP1 binds iron and functions as an aconitase. When cells are depleted of iron and under oxidative stress, iron is released allowing the apo-variant to bind to a non-coding RNA stem-loop structure of transcripts of iron metabolism genes, thereby regulating their translation or stability. Comparison of the structures of the iron containing aconitase variant and the apo-variant bound to RNA reveals large rearrangements of the IRP1 domains. Interestingly, many protein residues perform double duty by binding to either the metal cluster or the IRE RNA. To carry out both functions these regions of the protein structure are plastic, adopting different conformations that favor formation of the metal cluster or binding to the IRE RNA.

Carrie Wilmot, U. MN, presented the structure of an unusual fold for cytochrome P460. The P460 heme is the only one known in biology to withdraw electrons from an iron-coordinated substrate and has been characterized bound to two different proteins: the enzyme hydroxylamine oxidoreductase (HAO) and cytochrome P460. Determination of the structure of cytochrome P460 demonstrated the power of nonsynchrotron anomalous phasing. This structure was solved by single-wavelength anomalous diffraction on a Cr rotating anode with useful phasing power from 5 sulfur atoms in the protein, the iron of the heme and several solvent phosphates. The structure reveals a homodimer. Unlike most heme proteins, the structure of P460 is dominated by β-sheet. HAO also binds P460 but uses a different fold. Structural and mutagenesis studies show the cross-link between Lys70 and the 13'-meso carbon of heme that is responsible for the unusual spectral properties of P460. In contrast, tyrosine is linked to the heme in HAO enzymes, although questions remain about the exact nature of this chemical linkage. Cytochrome P460 is found in a number of human pathogens and perhaps plays a role in defense against neutrophil and macrophage host-generated NO. To investigate the possible role in NO detoxification, the structure of NO bound to cytochrome P460 was determined.

William Scott, UC Santa Cruz, told a tale of two ribozymes. The first tale illustrates that while truncation may be required to obtain crystals, one can remove too much. The original construct used to study the hammerhead ribozyme over a decade ago was too small, producing a crystal structure with some nucleotides critical for catalysis situated far from the active site. Working with a larger construct, containing an additional tertiary interaction and possessing significantly faster reaction rates, led to a structure where the catalytic residues identified by biochemical studies cluster in the active site. A large structural rearrangement is required to interconvert the core of these two structures that share the same sequence. In the second tale, Scott spoke of a structure that provides the first glimpse into how RNA might have replicated itself in the putative RNA world before proteins. The structure is of an *in vitro* selected RNA ligase, which illustrates an essential activity of an RNA polymerase. Cleverly, only active RNAs were selected by purifying the ligated products. The structure revealed two views of this ligase in the asymmetric unit. One view shows how tertiary and metal ion interactions stabilize a conformation with the substrate "docked" into the active site. Another view shows a more open conformation in which the substrate is "undocked." These structures provide interesting clues to the mechanism of action of the ribozyme; we look forward to additional structural snap-shots to view the pre-cleavaged structure.

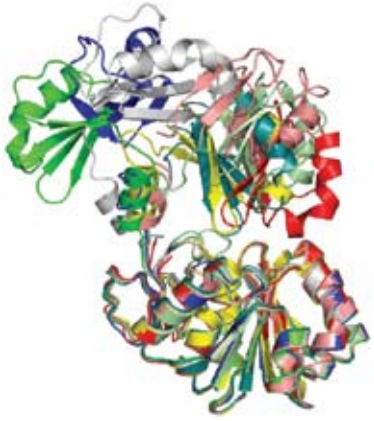
Laura Guogas, UNC, Chapel Hill was the last talk before the coffee break. She presented a structure of the C-terminal domain of a protein (TraI) involved in a multiprotein assembly (designated the relaxosome complex), which is responsible for conjugative DNA transfer (CDT). The structure of this region of TraI contains a bundle of alpha helices at its N-terminal region connected by a linker to a novel compact β-sheet core in the middle region. The C-terminal region of this protein fragment was disordered. The protein is a tetramer in the lattice, where the one α-helix from one subunit domain swaps into the compact β-sheet core of another subunit. Mutagenesis studies were presented that supported this domain swap architecture in solution and showed that the α-helical plus linker regions were essential for CDT. The role of the compact β-sheet and disordered region may be to interact with TraM, another member of the relaxosome complex.

After the coffee break, **Ya Ha**, Yale, discussed his structures of a rhomboid family intramembrane protease from *Escherichia coli*,

GlpG. This enzyme is unrelated in amino acid sequence to a mammalian intramembrane protease, γ-secretase, which is responsible for producing the amyloid β-peptide that forms plaques in the brains of Alzheimer's disease patients; however, GlpG probably has a catalytic mechanism similar to that of γ-secretase. First, he told us of the general architecture of the enzyme and discussed its "closed" conformation. GlpG is composed of six transmembrane helices. The amino terminus of a central helix is about 10 Å below the membrane surface, which creates an internal aqueous cavity inside the protein that opens to its extracellular side and contains many bound water molecules. Rhomboid protease family members have a large stretch of sequence between their first two helices that corresponds to a membrane embedded loop in the structure forming a lateral "gate" which may change conformation when substrate binds. The structure of GlpG supports the hypothesis that rhomboid proteases use a serine–histidine catalytic dyad. Later in his talk, he showed a second structure of GlpG in a more "open" conformation (which resulted from various soaking procedures), where a capping loop had been lifted, exposing the previously buried and catalytically essential serine to outside aqueous solution. A water molecule is observed in a putative oxyanion hole that is made up of a main-chain amide of the catalytic serine and two other conserved side chains. Furthermore, the capping loop movement appears to destabilize the side chain of a phenylalanine previously buried between two transmembrane helices and opens a side portal from the membrane lipid to the protease active site. Other structural rearrangements may be required to create a functional active site.

Allen Orville, BNL, also talked about active sites and mechanisms, but in his case it was that of FAD-dependent enzymes, particularly nitroalkane (NAO) and choline (CHO) oxidases. Structures for NAO included oxidized enzyme, the N5-nitrobutyl adduct, as well as several active site mutants and ligand complexes: all of these provided clues about the steps along the multistep reaction pathway of this enzyme. One of the newest structures presented included that of the C4α-OO(H) adduct of CHO which was generated *in situ* through FAD photoreduction, followed by reaction with O_2 from within the aerobic crystal; cryogenic conditions trapped the flavin-oxygen adduct and failed to establish the proper H^+ inventory on the surrounding residues required to yield H_2O_2. The audience was invited to utilize the single crystal microspectrophotometer being commissioned at beamline X26C at NSLS. This instrument will be able to collect complementary spectral data from the same crystal used for diffraction, as was done in some of the studies Orville presented.

Gerwald Jogl, Brown, impressed us with the sheer number of structures his lab had detemined of PrmA, the methyltransferase responsible for the trimethylation of multiple amino groups of ribosomal protein L11. Via a seemingly processive reaction mechanism the α-amino group of the N-terminal amino acid and the ε-amino group of two lysine residues, Lys3 and Lys39, are trimethylated. L11 is a universally conserved component of the large ribosomal subunit and an active participant in interactions of the ribosome with protein synthesis factors. It consists of a 23S rRNA binding C-terminal domain and an N-terminal domain responsible for direct ribosome-factor contacts. Therefore, the location of the L11 residues methylated by PrmA near the site of contact with elongation factors suggests a functional role for these methylations; PrmA has two domains connected by a flexible linker helix. The N-terminal domain is involved in recognition of L11 through formation of a β-sheet made of the two proteins. Incidentally, the C-terminal methyltransferase domain, which has a canonical class I methyltransferase fold, overlays nicely with that of HemK methyltransferase---a structure solved by Heidi Schubert and Chris Hill, our Salt Lake City local chairs! There are approximately 15 structures of PrmA (including mutants) from 11 crystals displaying 8 unique conformations of the protein. From these structures, it can be seen that the PrmA N-terminal domain is highly mobile relative to the catalytic domain. This high flexibility of the N-terminal substrate recognition domain is consistent with the unique requirement of PrmA to position its protein substrate in several different orientations in order to trimethylate the three amino groups.



Da Jia, Emory, finished the session. Whereas the previous talk was about a bacterial protein methyltransferase, here the topic was the structure of the catalytic domain of the mammalian cytosine DNA methyltransferase Dnmt3a in complex with C-terminal domain of its regulator, the methyltransferase-like Dnmt3L (a protein with a canonical class I methyltransferase fold but no active site). Both Dnmt3a and Dnmt3L are required for *de novo* methylation of imprinted genes in mammalian germ cells although the mechanism of targeted methylation has been unclear. The structure showed a heterodimer of Dnm3a-3L that further dimerizes through a Dnmt3a-3a interaction and forms a tetrameric enzyme complex with two active sites. Modeled B-DNA shows that the actives sites are approximately one DNA helical turn apart. Thus, the structure implies that two CpGs that are ~10 bp apart would have a greater probability of being methylated during genomic imprinting: statistical analyses of known methylated CpG patterns and biochemical studies have begun to corroborate this prediction. Interestingly, substitution of key residues in any of the protein interfaces in the tetramer eliminated its enzymatic activity.

We thank Hampton Research and Wyeth Instruments for their kind support of this year's "New Structures" session.

Carl Correll and John Horton

Image at left, from Gerwald Jogl: Least-squares superposition of eight PrmA conformations illustrating the enzyme's unusual interdomain flexibility.

Editor's note: Structures from Karl Volz and Gerwald Jogl were featured on the Cover -- see article, p.18.

1.03: Experimental Phasing with Longer Wavelength X-rays

From left: Cheng Yang, Nobuhisa Watenabe, George Sheldrick, Aiping Dong, Christophe Mueller-Dieckmann, Zbigniew Dauter, Ganapathy Sarma, John Rose, B.C.Wang, Manfred Weiss. *Photo courtesy of B.C. Wang.*

Owing to the fact that in the past few years, the collection of diffraction data at wavelengths longer than 1.5 Å has gained considerable popularity, the session attracted about 120 attendees. At such longer wavelengths the anomalous scattering of sulfur, phosphorous and other light atoms is significantly enhanced compared to when the data are collected at the typically used wavelengths around 1.0 Å. This has many implications in terms of, for example, possibilities for phase determination based on just the natively present sulfur atoms in proteins. However, since the sought for signals are very small, extremely accurate data collection is an absolute requirement

In first half of the session, chaired by **Manfred Weiss**, **John Rose**, U. Georgia, featured the description of an optimized beamline for long wavelength experiments at APS, built and operated by SER-CAT. This insertion device beamline appears to have significantly enhanced capabilities for long wavelength data collection over the previously used SER-CAT bending magnet beamline, which suffered from beam instabilities, which in turn made it less suitable for the type of experiments described. **Nobuhisa Watanabe**, Hokkaido U., Japan, described an easy-to-use loopless mounting procedure for the dry mounting of protein crystals, and showed that by mounting the crystals properly, a much higher data quality can be achieved reproducibly. **Christoph Müller-Dieckmann**, ESRF, France, demonstrated a case study on 23 protein crystals on which long wavelength data had been collected. In more than 90% of the cases, weakly bound ions such as sulfate or chloride could be picked up in an anomalous difference Fourier synthesis. Consequently, it was advocated that any structure determination ought to be complemented by a long wavelength data set. **Chen Yang**, Rigaku, then talked about the Rigaku chromium anode and the possibilities to carry out long wavelength work in the home laboratory.

In the second part of the session, **Bi-Cheng Wang** introduced **Zbigniew Dauter**, Argonne, who discussed radiation damage. Contrary to the widespread belief that long wavelengths are expected to cause more radiation damage because of more absorption, the experiment presented by Zbigniew provided evidence to the contrary. **George Sheldrick**, U. Göttingen, followed and presented new computational approaches, which are particularly relevant for data with phase extension and small signals, such as the ones obtained from sulfur SAD experiments. Practical examples were presented next. **Ganapathy Sarma**, UC San Diego, emphasized that the signal-to-noise ratio in data will at first increase with increasing redundancy but then degrade again if too many frames are included as a result of radiation damage. Finally, **Aiping Dong**, U.Toronto, presented a number of successful applications of the sulfur SAD technique using data collected from a chromium anode.

In summary, this session demonstrated that a technique advocated by only a few callers in the dark a few years ago, is now nearly in the mainstream of macromolecular crystallography.

Manfred S. Weiss and Bi-Cheng Wang

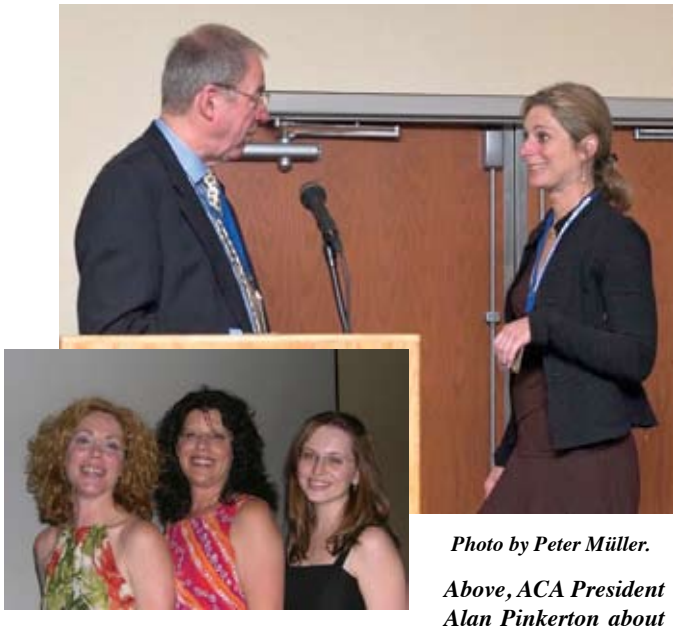


Photo by Peter Müller.

From left: ACA Administrative Director Marcia Colquhoun, Patti Coley, and Jennifer Curtice at the banquet. This experienced crew received much praise for their hard work and their success in problem-solving.

Above, ACA President Alan Pinkerton about to present the Elizabeth A. Wood Award to Lisa Randall.

In the center, Lisa Randall presenting her after-dinner Wood Award address. Across the bottom, ACA Past President Bob Bau presenting his Past-President's "speech," which consisted of an ode to the very much enjoyed meeting in Hawaii last year: a video and karaoke version of "Hawaian Love Song." Other banquet and reception shots, clockwise from upper left: Bill Duax; Jenny Glusker; table with Patti Coley, Marcia Colquhoun, S. N. Rao, and Judy Flippen-Anderson; under the table, Simon Teat and James Phillips; Tracy Arakaki and Giovanna Scapin* ; Jack Zack and Sue Byram* ; Gary Brayer, Ron Stenkamp and Leslie Williams; Richard Baxter and Matthias Zeller.*

**** All photos except those noted with asteerisk are by Peter Müller.***

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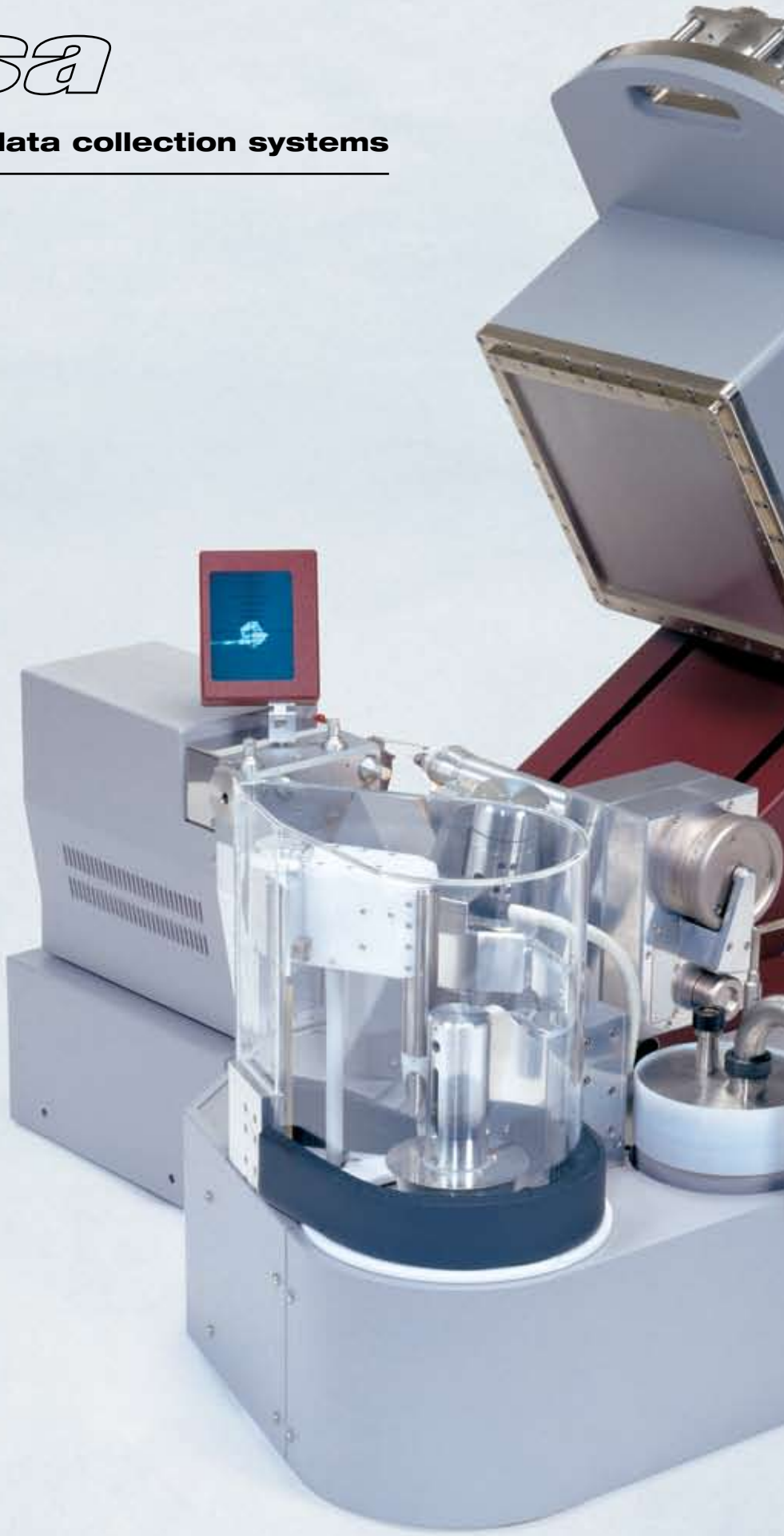

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From left: Rhiju Das, Paul Adams, Quan Hao, Greg Hura, Jack Johnson, Peter Zwart, Ethan Merritt, Ron Stenkamp, Elena Levin.

1.07: Computational Methods

This session highlighted the cross-fertilization of crystallographic analysis by structural descriptions from other fields. Two presentations demonstrated the possibility of obtaining initial crystallographic phases from a non-crystallographic starting point. **Quan Hao**, Cornell, reported progress in developing phases from a low- resolution model for the protein shape derived from small-angle scattering measurements. A 20Å envelope SAXS model for ADP-ribosylcyclase could be correctly placed into the crystallographic unit cell using a 6-dimensional grid search, essentially a demonstration of using a SAXS model for molecular replacement. Furthermore, simulations showed that if sufficiently high resolution crystallographic data are available, these initial low-resolution phases can be extended to high resolution by using a genetic algorithm to evolve internal structure for the electron density within the protein envelope. **Rhiju Das**, U.Washington, reported a spectacular case where no experimental model at all was needed for "molecular replacement." Instead the probe structure was a model developed *ab initio* by the Rosetta structure-prediction algorithm. Rhiju also showed that in less extreme cases the success rate of molecular replacement based on distantly related known structures can be improved by the use of Rosetta to create an optimized probe model.

The next presentations emphasized the incorporation of external physical models to describe protein flexibility in the course of crystallographic refinement. **Elena Levin**, U.Wisconsin, presented recent work on the use of elastic network models to generate an ensemble of multiple structural models that jointly represent harmonic and anharmonic displacements in the crystal. Results showed that free-R factors could be reduced by the use of multi-copy refinement in cases using test and real data. The pros and cons of the method were explored in several questions from the audience. **Ronald Stenkamp**, U.Washington, presented work still in progress on comparing the refinement of ensemble models to the refinement of a single model supplemented by a multi-group translation-libration-screw model for harmonic displacements.

Jack Johnson, Scripps, described the synergistic use of electron microscopy and x-ray crystallography to characterize the physical basis for conformational changes in viral capsids. **Greg Hura**, Lawrence Berkeley Lab. (LBL), described the SIBYLS combined MX/SAXS beamline at the ALS. This included recent work to increase the automation of SAXS data collection, the use of SAXS profiles to identify potential protein folds, and efforts to create reliability scores for the results of SAXS data analysis. **Peter Zwart**, LBL, gave a background to the problem of twinning in crystallography and described tools in the PHENIX software. These included a program called **phenix.xtriage** for identifying twinning from the diffraction data, and **phenix.refine** for refinement of structures taking twinning into account. Peter described unique features in **phenix.refine** such as the use of twinning data with TLS and anomalous scattering parameter refinement. Results showed the importance of the correct handling of twinning in structure solution in terms of R-factors and electron density maps.

Paul Adams and Ethan Merritt

Sue Byram, Roger Kornberg, and Chris Hill.

SP.02:Plenary Nobel Lecture

The final morning of the conference began with a plenary lecture by Nobel Laureate **Roger Kornberg**. Kornberg was awarded the 2006 Nobel Prize for Chemistry for his studies of eukaryotic transcription. Most notably, his lab determined the crystal structure of RNA Polymerase II (RNA Pol II), the enzyme that copies DNA to mRNA, which is the essential intermediate in the biosynthesis of proteins. Not surprisingly, the large lecture room was full and the presentation generated considerable excitement. Thanks are due to Sue Byram and Bruker AXS, whose generous support made this lecture possible.

Nobel Lecture, cont'd.

While a postdoc in the Laboratory of Molecular Biology of the Medical Research Council at Cambridge, England, Kornberg discovered nucleosomes, the fundamental packaging unit of DNA. Nucleosomal structure presents a substantial barrier to polymerases, such as RNA Pol II, and Kornberg's subsequent career at Stanford University has focused on understanding how the DNA is copied to mRNA and how this process of transcription is regulated. His lab played a leading role in elucidating the identity and roles of general transcription factors and demonstrating that the transcriptional mechanisms are conserved between yeast and human. These included identifying the large (1 MDa, 20 subunit) mediator complex, which links gene-specific proteins with the general transcriptional apparatus centered around RNA Pol II. Over a period of more than two decades, Kornberg pursued crystallographic studies of Pol II, an effort that required considerable effort and creativity at every step, including sample preparation and purification, crystallization, phasing, and structure determination. Eventually, the 10 subunit, 500 kDa enzyme structure was revealed at near atomic resolution.

Notably, Kornberg's talk emphasized recent new results, including the role of the trigger loop, which moves upon binding of a cognate ribonucleotide against the DNA template to make reinforcing interactions that enhance both substrate specificity and catalysis. Various complex structures were described that together show the path and relative positions of DNA and RNA, the mechanisms by which the different DNA and RNA strands are directed in their separate directions, and the mechanism by which transcription factor IIB (TFIIB) regulates transcription initiation. Combination of the available x-ray crystal structures and electron microscopic reconstructions allowed construction of a composite model for the intact initiating Pol II holoenzyme, comprised of 1.5 MDa and 17 protein subunits. The presentation left the audience buzzing with excitement about the extraordinary science that has been accomplished.

Kornberg's talk was naturally followed by

1.08: Large & Difficult Structures

From left: Marc Allaire, Venki Ramakrishnan, Chris Hill, Dan Anderson, Bill Royer, Christopher Lima.

The five excellent presentations included talks by: **Bill Royer**, U. Mass. Medical School, on erythrocruorins, which are 180 subunit, 36 MDa extracellular respiratory complexes of annelids (includes earthworms and leeches); **Dan Anderson**, UCLA, on the vault protein assembly, which is the shell of a 700 x 400 x 400 Å, 13 MDa ribonuclear protein complex of eukaryotic cells that is comprised of 96 copies of the protein and may function in innate immunity; and **Marc Allaire**, BNL, on a relatively small snake venom disintegrin structure determination. Phasing presented considerable challenges in this work; molecular replacement, isomorphous replacement, and anomalous scattering were used. The presentations by **Chris Lima**, Sloan-Kettering, and **Venki Ramakrishnan**, MRC Lab. of Molecular Biology, Cambridge, each of which had an obvious intellectual connection with Kornberg's talk, will be outlined in a little more detail here.

Chris Lima described structural and enzymatic studies on the exosome from human and yeast. Exosomes are 300 kDa complexes of 9, 10, or 11 protein subunits that function in the processing and degradation of RNA. Technical highlights included the comprehensive use of bacterial coexpression systems to develop the protein complexes; the coupling of structural and biochemical studies; the challenges of phasing with a multi-heavy atom cluster; and the importance of sequence markers such as selenomethionine for the interpretation of medium resolution maps. The structure revealed that some subunits wrap extended arms around their neighbors, which explains why coexpression rather than reconstitution from separate subunits is critically important. A particularly surprising finding was that although eukaryotic exosomes share some overall architectural similarity with archaeal exosomes including a hollow structure with sequestered hydrolytic sites, the path taken by substrates into the archaeal and eukaryotic exosome complexes appears to be different.

Finally, **Venki Ramakrishnan** described his remarkable successes with determination of ribosome structures. High resolution structures of 30S subunits in a variety of complexes have explained much about ribosome mechanisms, especially the mechanism of decoding, which is the process by which mRNA is faithfully interpreted by tRNA molecules that deliver the appropriate activated amino acid residue. This has long been recognized as a notable challenge of protein synthesis that requires interactions of inherently low affinity to define a high level of substrate specificity while also accommodating redundancy and alternative interactions (wobble) in the recognition of 61 codons by a smaller number of tRNA molecules. Interestingly, the mechanism of decoding has some parallel with the trigger loop/helix mechanism of RNA Pol II, because binding of a cognate substrate induces a conformational change (in this case flipping out of ribosome nucleotides) to make additional interactions that reinforce the codon-anticodon interaction and thereby ensure specificity. Also described was the 2.8 Å resolution structure of the 70S ribsome complex. This is the highest resolution 70S structure currently available and reveals a remarkable level of detail - even including solvent coordination geometry for Mg2+ ions. Importantly, this structure in complex with mRNA and tRNA explains how slippage of mRNA in the ribosome is avoided. It also appears to resolve a controversy regarding the mechanism of peptidyl transfer and shows that, at least to some extent, protein does contribute directly to this reaction.

cont'd, next page

1.08: Large & Difficult Structures, cont'd.

The audience was receptive to the implicit messages of this session that crystallography is a very powerful technique for addressing fundamental questions of mechanism and that crystallographers should attack scientifically ambitious targets. It was also striking that the greatest insights came from relatively high resolution data. Even megadalton complexes work at the level of interactions between atoms, and the key to understanding these processes is availability of crystals of relevant complexes that diffract to high resolution. This may seem like a trivial conclusion, but one worth remembering for those of us who have struggled excessively with trying to interpret marginal diffraction from exciting projects; the answer is often – get better crystals.

Chris Hill

We gratefully acknowledge Area Detector Systems, Corp, Array BioPharma, Inc., Art Robbins Instruments, Boehringer Ingelheim Pharmaceutical Research Inst., and Pfizer, Inc. for their partial support of this session.

From left: Peter Turner, Xiaolei Ma, Bruce Noll, Yingssu Ttsai, Oana Luca, Michael Ruf, Dusan Turk.

3.01 General Interest I

General Interest sessions are home to presentations that appeal to a broad audience or that do not readily fall into another category. This year the talks were about macromolecular crystallography, small molecules, instrumentation, and software.

Yingssu Tsai,UCLA, began the session by describing the structure of the CsoS1A component of the carboxysome shell of *Halothiobacillus neapolitanus*. This was followed by **Xiaolai Ma**, Case Western Reserve, and a description of diatomic ligand discrimination by soluble guanylyl cyclase. Filling in for a last-minute cancellation was **Oana Luca**, an undergraduate at Worcester Polytechnic Inst. Oana attended the 2007 ACA Summer School, and described her experience there, which included three structure determinations. **Dusan Turk**, Josef Stefan Inst., Slovenia, offered a view of PURY, a database built upon the Cambridge Structural Database that can be used to verify the geometry of a fragment built for structure refinement. **Joerg Wiessman**, Incoatec GmbH, Germany, then presented the latest developments in x-ray optics and microfocusing sources. **Michael Ruf**, Bruker AXS, demonstrated start-to-finish automation for small-molecule structure determinations and **Peter Turner**, U. Sydney, Australia, closed with a report of successful efforts using web services for remote access to laboratory instrumentation.

Bruce Noll and Allen Oliver

From Yingssu Tsai: CsoS1A is a major small shell protein of the Halothiobacillus neapolitanus carboxysome. The structure of the CsoS1A hexamer is shown on the top, with each protein molecule colored differently. The CsoS1A hexamer was found to form a layer, shown in the middle, as observed in previous structures of shell proteins. The layer of carboxysome shell protein is thought to form the faces of the carboxysome, as shown in cartoon form on the bottom. Adapted from Y Tsai et al. (2007) PLoS Biol 5, e144, and TO Yeates et al. (2007) Biochem. Soc. Trans. 35, 508–511.

From Left: Carroll Johnson, Henk Schenk, Ryoji Kiyanagi, Werner Kaminsky, Regine Herbst-Irmer, Bruce Noll, Allen Oliver.

3.02 General Interest II Speakers

3.02 General Interest II

Regine Herbst-Irmer, U. Göttingen, Germany, described ways to deal with non-merohedral twinning for both small molecule and macromolecular studies. Use of the program **cell_now** was demonstrated. **Ryoji Kiyanagi**, Argonne, demonstrated his software which employs an alternative calculation method to reconstruct neutron/electron density distributions. This was demonstrated by highlighting hydrogen positions in a water-doped $YBaCeO_3$. **Carroll Johnson**, ORNL, gave a very in-depth and mathematical talk discussing an alternative method of formulating space groups using Riemann-Finsler geometries. **Henk Shenk**, U. Amsterdam, gave a delightful talk discussing polymorphism in chocolate and how it might be controlled to give the more desirable β–V form. **Bruce Noll**, U. Notre Dame, presented his research on the temperature dependent phase transformation of iron nitrosyl tetraphenylporphyrin. The session concluded with a very visually-oriented presentation by **Werner Kaminsky**, U. Washington, who described the various applets and software that he has programmed and found.

Allen Oliver and Bruce Noll

From Werner Kaminsky: The amethyst aggregate was 'grown in silico'; computer simulated virtual objects like this were created using the WinXmorph program. This software, including the shown example and others, is available free of charge from http://cad4.cpac.washington.edu/WinXmorphHome/WinXmorph.htm. W. Kaminsky, J. Appl. Cryst. (2007). 40, 382–385.

From left: John Badger, Tim Rydel, Doug Davies, John Barker, Giovanna Scapin, Ping Chen, Rick Bott, John DiMarco.

4.01 Impact of Crystallography in Industry

This session focused on the many ways crystallography is used in diverse commercial pursuits and the development of crystallographic tools to support these pursuits. The presentations featured characterization of industrial enzymes with potential for detergent use; development of agricultural agents to improve crop resistance and yield; and three facets of drug discovery: fragment-based screening, small molecule polymorph characterization, and structure-based drug design (SBDD). During the concluding roundtable discussion, several questions related to fragment-based screening were asked. In addition, Helen Berman, RCSB, asked why there were not more x-ray crystal structures from industrial members deposited. The primary reason given was the lack of time to refine historical structures to completion. A couple of potential solutions, which included an intermediate repository for partially refined structures available for completion by the crystallographic community, were briefly discussed.

Ping Chen, Pfizer, LaJolla, described how structural information played a crucial role in the development of a potent and selective inhibitor of CHK1, a serine/threonine protein kinase that plays an essential role in the regulation of S-phase and G2 checkpoints. Chen and co-workers identified the binding pocket in the co-crystal structures that led to the design of inhibitors with significant improvement both in potency and selectivity for the CHK1. She emphasized that because the drug design process is iterative, in order to provide timely structural information it was necessary to create several constructs of CHK1, using molecular biology to identify the ones that would yield high quality crystals. She also emphasized the importance of establishing a universal SBDD tool.

John Barker, Evotec, introduced a fragment screening strategy for using small molecule fragments for drug discovery designated FBDD. He described a screening strategy whereby binding followed by confocal microscopy could observe individual binding events induced by displacement of dye labeled inhibitor. He showed how x-ray structures could sometimes be determined from soaking different compounds into existing crystals of target enzyme.

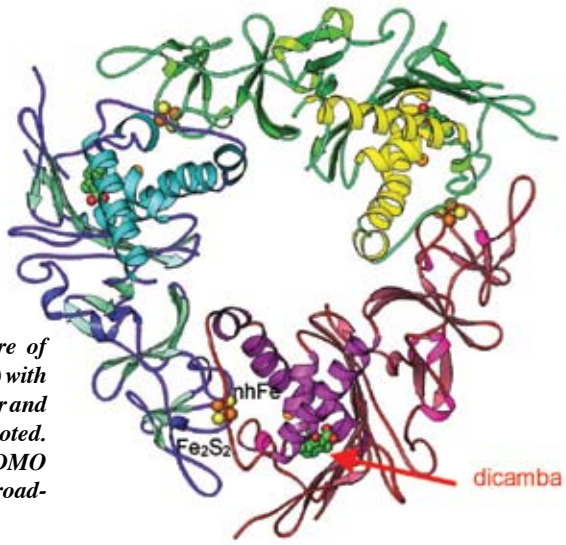
Doug Davies, deCode, followed with a presentation that also was based on fragment screening but in this case the fragments came from a library of natural metabolites designated "Fragments of Life." The target molecule was leukotriene A4 hydrolase which is a zinc metalloenzyme. The three-dimensional structure showed a large elbow shaped channel leading to the active site. Several different fragments were seen to bind at different sites in the channel suggesting again how a candidate compound could be assembled to produce the desired high affinity and specificity for a drug candidate.

John Badger, ActiveSight, described their efforts to automate co-crystal structure determinations for large numbers of related datasets with the MIFit software. A key component of this effort was to include expert decision making processes in the

4.01: Impact of Crystallography in Industry, con't

automation software and thereby minimize the user intervention required to accomplish co-crystal structure determinations. The automation pipeline now includes data processing and ligand placement in addition to refinement. MIFit is used to support the fragment screening and early lead discovery services offered by ActiveSight.

Tim Rydel, Monsanto, described four projects, three pertaining to insect control and one related to herbicide tolerance, all of which benefited from the use of protein crystallography. In the area of insect control, the crystal structure of the Bt Cry protein Cry3Bb1 was used to develop a variant with commercial level corn rootworm activity that is currently in Monsanto's YieldGard Rootworm corn. The Cry1Aa crystal structure aided the design of the Cry1A.105 hybrid Cry1 protein, which has enhanced activity versus key lepidopteran pests of corn, and the crystal structure of Cry1A.105 has facilitated its regulatory submission. The crystal structure of patatin, a lipid acyl hydrolase from potato tubers with corn rootworm activity, revealed novel structural features that facilitated an understanding of its biochemistry, and allowed an active patatin permutein to be developed. Finally, crystallography on the DMO terminal oxygenase, which degrades herbicidal dicamba, revealed key structural details about this herbicide tolerance enzyme.



From Tim Rydel:: The structure of dicamba mono-oxygenase (DMO) with dicamba bound. The Fe_2S_2 cluster and non-heme iron (nhFe) site are noted. Monsanto is interested in using DMO for herbicide resistance to the broad-leaf herbicide dicamba.

John DiMarco, Bristol-Myers Squibb, showed how single-crystal studies can be used to design and monitor a complicated manufacturing process. In the final processing stages of dasatinib, seven crystal forms were encountered, but only one had the desired form. Several crystal forms were observed to interconvert both through dissolution-recrystallization and topotactically (single crystal to single crystal). The topotactic relationships between some of the forms were established using single crystal analysis of transformations due to desolvation. The seven crystal forms comprised the basis for predicting powder x-ray diffraction patterns. They were correlated with subsequent Raman and near IR techniques and used to design and monitor a manufacturing process to produce the desired crystal form.

Giovanna Scapin, Merck, presented nice examples of how SBDD was used to generate lead molecules with the necessary potency and specificity for three different classes of enzymes: PTP1b phosphatase, DDP-IV peptidase, and p38 kinase. In the case of p38 kinase, x-ray crystal structures showed how the hinge region was able to adopt an alternative conformation upon inhibitor binding. Specificity is due to the inability of off-target kinases with different amino acid sequences to adopt this alternate protein conformation. For PTP1b, structural biology identified the binding mode of two apparently equivalent classes of potent inhibitors and guided the decision about which class was the most suitable for achieving selectivity against the closely related T-cell phosphatase. In the DPP-IV program, structures with α- and β-amino acid inhibitors guided the molecular modeling and chemistry efforts in the design of novel, structurally diverse molecules, which retained the potency and the *in vivo* properties of the parent compounds.

Rick Bott, Genencor, discussed the characterization and development of commercial enzymes for potential detergent use and presented the x-ray crystal structure of a novel SGNH hydrolase. He also discussed the history of the subtilisin family of industrial enzymes, showing how patents have traditionally focused on advantageous mutations.

Rick Bott

5.01: Non-Ambient Crystallography

Several speakers discussed phase transitions by variable temperature diffraction (laboratory x-ray, synchrotron x-ray, and neutron); others presented ways to augment experimental set-ups. Alloys, ceramics, and organic/inorganic compounds with a wide range of potential applications, such as thermal barrier coatings, microwave dielectrics, and composites in materials with zero thermal expansion were used in the studies.

Scott Speakman, MIT, discussed *in-situ* diffraction studies of Ni-Al alloys used for thermal barrier coatings in high temperature applications. Large volume changes associated with phase transitions of the Ni-Al alloys can lead to the failure during service. His study focused on the effects of Pt alloys and Hf doping and was designed to determine quantitative phase fractions at different temperatures. It was not possible in all cases to quantitate the different phases that occur because of large grain sizes. This was especially true when the samples partially recrystallized at higher temperatures.

Davide Viterbo, Università del Piemonte Orientale, Italy, reported on a novel experimental set-up for simultaneous *in-situ* Raman/high resolution x-ray powder diffraction diffraction (XRPD) measurements. This system has been developed and is located at the Swiss-Norwegian Beamline at the European Synchrotron Radiation Facility (ESRF). The new experimental set-up has been tested on three solid-state transformations.

Jana Bezjak, Institute Jozef Stefan, used XRPD to observe three structural phase transitions that occur below 1400°C for the compound $Ba_4Nb_2O_9$. The authors found the compound $Ba_4Bn_2O_9$ is of interest due to its similarity to the ternary compound $Ba_6WNb_2O_{14}$, which is reported to have the hexagonal-perovskite related structure. Hexagonal perovskites are of interest as potential components in the wireless communication industry.

Roger Willett, Washington State U., presented research on the compound $[(C_6H_5)_3/CH_3P]Cu_3Br_4$ which experiences a continuous order-disorder transition between 90°K and room temperature - while retaining the $P2_1/n$ space group in the crystal structure. The atomic displacement parameters of the Cu atoms are large and suggest that the disorder is occurring at this site; the Br atoms do not undergo major reorganization.

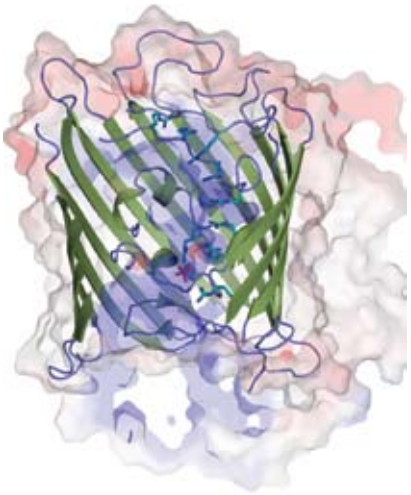
Amy and Claudia. Both photos on this page by Cora Lind.

Amy Gindhart, U. Toledo, at left, received the Materials SIG's **2007 Margaret C. Etter Student Lecturer Award** from session organizer **Claudia Rawn**. She talked about her variable temperature x-ray and neutron powder diffraction studies. These techniques were used to study the thermal expansion and phase transitions in $AA'W_3O_{12}$ ($A=Mg^{2+}$, Zn^{2+}; $A'=Zr^{4+}$, Hf^{4+}) samples. The orthorhombic polymorph of these materials exhibits negative thermal expansion (NTE) behavior.

From left, standing: Mateusz Pitak, Milan Gembicky, Roger Willett, Davide Viterbo, Scott Speakman. In front: Jana Bezjak, Claudia Rawn, Amy Gindhart.

Milan Gembicky and **Mateusz Pitak**, SUNY Buffalo, described small molecule Laue diffraction for time-resolved (TR) experiments. The experiments were performed with the NW14 new insertion device beamline at the Advanced Ring (PF-AR) at the Photon Factory (KEK), Tsukuba, Japan, which is fully dedicated to TR experiments. Accumulated exposure times were on the order of 1-5 ns per CCD frame. Careful data analysis led to Rf-factors of 5-6% which is a relatively good result for these types of experiments. Use of the Laue technique is essential in sub-microsecond TR experiments but requires further testing.

Claudia Rawn



From Trevor Moraes, session 1.04: OprP is a phosphate specific channel that resides in the outer membrane of the Gram negative bacteria Pseudomonas aeruginosa. The arginine ladder in OprP functions to attract anions through its electropositive channel towards a coordination site where phosphate is selectively bound. The 9 arginine residues in OprP that participate in anion transport are illustrated and shadowed by the electrostatic potential calculated by APBS and displayed by Pymol. Moraes, T.F., Bains, M., Hancock, R.E. & Strynadka, N.C. Nat Struct Mol Biol 14, 85-7 (2007).

5.02: Crystallographic Mineralogy, Real Crystals, Extreme Conditions

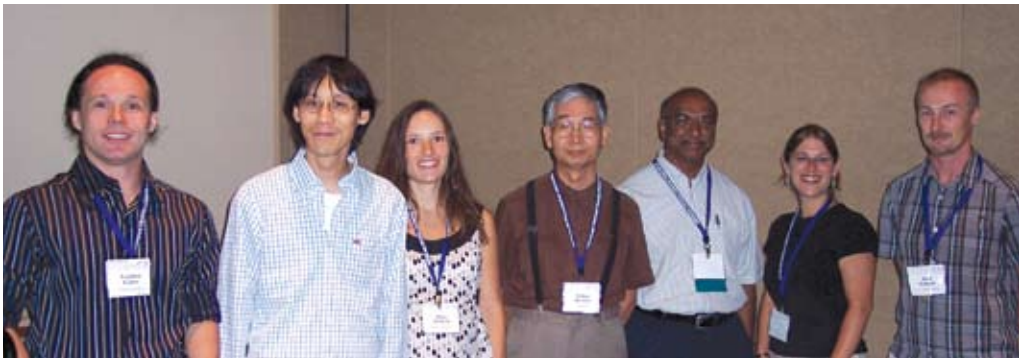
The session hosted a diverse mix of research; studies concerned the deep earth and also the surface of Mars; there was discussion of manmade problems in acid mine drainage, and also manmade benefits in materials with useful properties. An underlying theme was that even in seemingly simple chemical compounds, the crystallography can be complex and difficult at the conditions of interest.

In front, from left: Chris Tulk, Lee Groat, Gary Enright, Claudia Rawn, Bob Bau, Davide Viterbo; in back: Bryan Chakoumakos, Ron Peterson, George Lager, Ton Spek, Claude Lecomte, Hongwu Ya, Cora Lind. *Photo by Bill Duax.*

George Lager, U. Louisville, gave an overview that explored the crystallography of the major earth materials at high pressure and temperature that would be encountered in a descent to the center of the earth. Changes in stable crystal structures as pressure and temperature increase cause many global earth processes. Some earthquakes are caused by phase transitions with large volume changes, and devolatization reactions can promote volcanism. Detailed structural studies of crystals at high pressures and temperatures are key to understanding many large scale planetary processes. **Ron Peterson**, Queen's U., gave a review of his group's current research on metal sulfates, describing their implications for mitigating the environmental impact of acid mine drainage as well as the role they play in shaping the surface of Mars. Diffractometry with carefully controlled temperature and humidity are necessary experimental tools. **Chris Tulk**, ORNL, showed how combined Rietveld and PDF studies with synchrotron x-rays can be used to elucidate the disorder of the guest atoms in the noble gas hydrates. Disorder and guest/host inclusion compounds have long presented problems that now can be tackled by a combination of traditional and new analysis methods.

An eclectic assortment of other talks featured high pressure studies of metal hydroxides, photocrystallography of magnetic molecules, and the crystallographic response to isomorphism and polymorphism in both unusual minerals and technologically significant materials. A goal of this session was to re-institute an ongoing mineralogy component in the ACA program, something that used to be common in the past but somehow lost favor in recent years. We hope sessions like this one can rekindle interest, and attract mineralogical crystallographers to ACA meetings. The European Crystallographic Association has had a special interest group in mineralogical crystallography for many years.

Bryan Chakoumakos & Lee Groat



From left: Leighton Coates, Julian Chen, Flora Meilleur, Nobuo Niimuro, P. Thiyagarajan, Zoë Fisher, Paul Langan.

6.01: Neutron Macromolecular Crystallography

New structures were featured in this session, organized by **Paul Langan**, LANL, and **P. Thiyagarajan**, ANL. Several fresh faces to the neutron protein crystallography community were heard from: the keynote speaker **Julian Chen**, Goethe U., Frankfurt, presented the structure of diisopropyl fluorophosphatase from *Loligo vulgaris*, **Pavel Afonine**, LBNL, spoke about the structure of human aldose reductase, **Zoë Fisher**, LANL, about the structure of photoactive yellow protein from *Halorhodospira halophila* and **Marat Mustyakimov**, LANL, about the structure of polyamine-free, and low pH, left-handed Z-DNA.

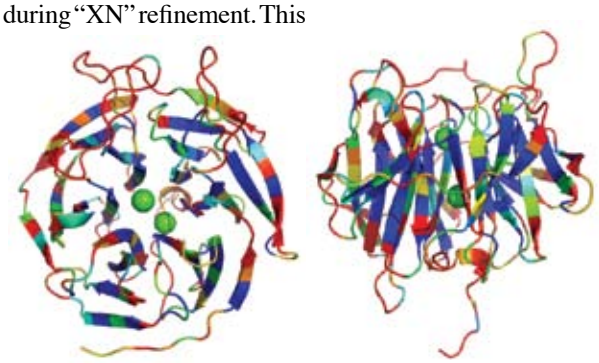
Other presentations (by familiar faces to NMC) described highly sophisticated experiments on previously studied proteins. **Nobuo Niimura**, Ibaraki U., presented exquisite nuclear density maps from neutron crystallographic titration studies of porcine cubic insulin and bovine pancreatic ribonuclease A, revealing changes in the protonation states of some important ionizable residues. **Flora Meilleur**, North Carolina U. and SNS, explained that her large xylose isomerase crystal, the planned subject of her talk, was damaged during data collection. Instead, she presented preliminary data on the rapid data collection (14 hours) on deuterated rubredoxin with and without labeled residues. These data will be used by **David Langs** and his colleagues from the Hauptman-Woodward Institute to investigate the feasibility of using SIR with H/D exchange to phase new protein structures as described in their poster **TP185**.

6.01: Neutron Macromolecular Crystallography, cont'd.

Finally, **Leighton Coates**, ORNL, described how new structure refinement software from the Macromolecular Neutron Crystallography (MNC) consortium had greatly improved the structure of endothiapepsin. Deuteration and its use in providing mechanistic insights into haloalkane dehalogenase from *Xanthobacter autotrophicus* was the subject of a poster related to this session, **SP187**, by **Xuying Liu** and colleagues, U. Toledo and LANL.

An emerging theme in most of the talks, and one that generated a great deal of excitement and discussion afterwards, was the use of both x-ray and neutron diffraction data during "XN" refinement. This approach, originally developed by Wlodawer and Hendrickson many years ago, has the advantage of increasing the data-to-parameter ratio and hence the accuracy of the structures. In its more recent application -to the five structures presented in this session, joint XN refinement has been combined with cross-validated maximum likelihood refinement in a patch for the program **CNS**, called **nCNS** and in new features of the program **PHENIX**. These software advances are part of the computational tools for NPX being developed by the MNC consortium between LANL and LBNL. The NIGMS-funded MNC freely distributes this software. Those wishing guidance in downloading and using **nCNS** can contact **marat@lanl.gov** or **langan_paul@lanl.gov** and those wishing guidance in downloading and using **PHENIX** can contact **PAfonine@lbl.gov** or **PDAdams@lbl.gov**.

Paul Langan and P. Thiyagarajan



From Julian Chen: top (on the left) and side views of the structure of diisopropyl fluorophosphatase (DFPase) illustrating residues involved in backbone hydrogen / deuterium exchange. Residues are colored from unexchanged (blue) to fully exchanged (red). The two associated calcium ions are shown as green spheres.

Photo by Victor Young.

Paval Juhas, Jae-Uyuk Her, Bob vonDreele, Ashfia Huq, Jason Hodges, Abe Clearfield, Eugene Cheung, Peter Stephens.

7.01 SDPD (Structure Determination from Powder Diffraction): Getting Better and Better:

This full day session highlighted the advances in the field of structure determination from powder diffraction data and its application in various materials related research. **Bill David**, ISIS, RAL, led with an introduction to a hybrid Monte Carlo search algorithm developed to solve a number of different crystal structures. He also described the use of a system for distributed parallel computing 'GRIDMP' using existing desktop computing resources at ISIS. **Chris Gilmore**, U. Glasgow, discussed the use of the Maximum Entropy (ME) method for electron diffraction data to solve crystal structures of Zeolites which are of importance to his collaborators at ExxonMobil. This method, using density building functions and density histogram-matching coupled with ME and likelihood analysis, can also be used for structure solution from powder diffraction. Aromatic carboxylates, trimellitates which are impurities in the commercial synthesis of terephthalic acid and other aromatic acids, are the compounds of interest to **James Kaduk**, INEOS Technologies. He determined the crystal structure of several of these compounds using powder data, and examined the bonding using quantum chemical calculations. *The crystal structure of kryptonite/jadarite* was presented by **Pamela Whitfield**, NRC, Canada. A new mineral, $LiNaSiB_3O_7(OH)$, matching the unique chemistry of "Kryptonite" as described in the film Superman Returns was identified in a mine in Serbia. Unlike the fictitious compound which is the source of Superman's powers the real mineral is white and harmless. The crystal structure was solved by simulated annealing in TOPAS (Bruker-AXS). VASP *ab-initio* optimization was used to validate the structure and to locate the H atom.

7.01 SDPD, con't.

Peter Stephens, SUNY, Stony Brook, gave an enlightening talk on molecular based magnets synthesized in J.S. Miller's laboratory at U. Utah. The structures of several magnetic salts of transition or alkali metals and TCNE, [$C_2(CN)_4$] were solved using the high resolution powder diffraction beamline at NSLS, BNL; the structural information aided understanding of their magnetic behavior. **Abraham Clearfield**, Texas A&M, followed with another informative presentation on the use of titanium silicates to sequester and immobilize nuclear waste such as Cs-137, Sr-90 and actinides Pu and Np. He explained that the use of powder x-ray and neutron diffraction along with *in-situ* x-ray diffraction revealed both the structural origin of selectivity and the mechanism of exchange reactions. **Eugene Y. Cheung**, TransForm Pharmaceuticals, shifted gears and described the use of powder diffraction as a structure solution technique in the pharmaceutical industry, especially for polymorphs of amides. The emerging field of high resolution powder protein crystallography was presented by **Robert Von Dreele**, Argonne. He described the powder patterns from proteins, which show remarkable sensitivity to experimental conditions such as temperature, pressure, pH, solvent composition, ligand binding and radiation effects without significant changes in protein folding. This suggests a way to develop techniques to overcome the overlap problem of powders and enhance the ability to extract intensities, a crucial step towards structure solution of proteins. He also presented his efforts in fast data collection at APS using image plate detectors to avoid radiation damage of the sample. **Jason Hodges**, ORNL, Spallation Neutron Source (SNS), described the future prospects of structure solution from neutron powder diffraction at POWGEN3, a diffractometer currently under construction at the SNS at ORNL. He presented an overview of the resolution achievable at this instrument and the degree of complexity of the crystal structures that can be analyzed. **Jae-Hyuk Her**, SUNY, Stony Brook, was presented with an **Etter Student Lecturer Award** for his work on the development of the ME Program for Powder Diffraction (MEPPD) to solve disordered crystal structures and solvent scattering problems. **Pavol Juhas**, MSU, described a very different technique to get structural information about non-crystallized molecules and nano-materials based on the atomic Pair Distribution Function (PDF) technique. He described the European-Soccer-League-inspired ***Liga*** algorithm which was successfully used to solve the molecular structure of C_{60} from distances obtained from neutron PDF data. This suggests tantalizing options for studying structural properties of a vast number of systems where periodic order is not present and conventional crystallographic methods cannot be applied.

Ashfia Huq

9.01: USAXS/USANS

From left: Andrew Allen, V. Siva Kumar, Trevor Willey, Jan Ilavsky, Dale Schaefer, Kenneth Littrell, Govidarajan Muralidharan, Fan Zhang.

The session provided an excellent review of the current techniques and instrumentation as well as an overview of a wide range of applications. **Jan Ilavsky**, APS, Argonne, presented *USAXS Facility at Advanced Photon Source for Complex Microstructure Studies in Materials Science*, an overview of USAXS and USANS techniques and discussed in detail capabilities of the APS USAXS instrument, the dominating USAXS facility in the USA. Ultra-Small Angle Scattering (USAXS) instruments, mostly with Bonse-Hart design, extend the measured small angle scattering range to scattering vectors smaller than 10^{-3} Å^{-1}. USAXS instruments provide data in a single, ~ 20 minute experiment with over 4 decades range of scattering vectors (from 10^{-4} to 1 Å^{-1}), and over 8 decades of scattering intensities. The USANS extends this range down to about 10^{-5} Å^{-1} but with a smaller range of scattering vectors and intensities. These techniques extend the SAS range to scatterers from nanometers to micrometers.

Dale Schaefer, U. Cincinnati, introduced the audience to the problem of developing new and better encapsulants for flavors in the food industry. In this case the use of USAXS provided unique data necessary the for development of a novel method of flavor encapsulation that enables the number of flavors in food preparation to be reduced. This provides for a significant cost savings. He also presented *Small-Angle Scattering Studies of the Hierarchical Structure of Reinforcing Fillers* on the hierarchical structure of polymer fillers and the need for the extended size range accessible by USAXS techniques. In order to access the size of interest, one needs to combine the 4-decades size range accessible using USAXS with either USANS or, if possible, dynamic light scattering. Only with characterization spanning five or more decades can an understanding of the behavior and properties of these materials be developed.

Trevor Willey, Lawrence Livermore Nat'l Lab., presented *Void Distributions in Temperature-Cycled Insensitive High Explosives*,

which documented the need to combine a variety of techniques in order to understand ratchet growth in these interesting materials. Extensive study, including *in situ* measurements showed that the most complete characterization of the voids related to ratchet growth, can be achieved by combining tomography techniques for voids larger than a micron with USAXS and USANS techniques for smaller voids. **Govindarajan Muralidharan**, ORNL, then discussed USAXS and USANS techniques for studies of precipitates in special steels which have applications in nuclear powerplants. **Andrew Allen**, NIST, presented two examples of the use of USAXS in studies of materials for biomedical applications. He described details of custom made instrumentation - using a flow cell, which enables *in-situ* studies of formation of anisotropic particles in extended and constricted enviornments.

9.02: Surface & Interface Characterizations

This session provided a comprehensive overview of the use of scattering techniques to characterize surface chemistry, materials, and physics of nano-objects on substrates in various environments, including reactive gas, vacuum, and aqueous solutions. Developments and applications of reflectivity and grazing incident small/wide angle x-ray scattering techniques were discussed.

Dale W. Schaefer, U. Cincinnati, talked about his recent study on low-dielectric materials characterized by x-ray/neutron reflectivity in conjunction with grazing incident x-ray scattering (GIXS). He discussed variations in physical/chemical properties and molecular-level-structures as a function of ratios of starting materials. **Changyong Park**, Argonne, described his phase resonant anomalous x-ray reflectivity (RAXR) technique and the Fourier synthesis method he used to extract element-specific density profiles. He demonstrated applications of this technique to studies of adsorptions of rare earth metal ions on mineral surfaces in aqueous environments. **Randall Winans**, Argonne, reported on *in-situ* grazing incident SAS studies of size-selective nano-cluster catalysis and catalytic reactivity in gas environments such as hydrogen and/or carbon monoxide at about atmospheric pressure. Shapes of aggregated clusters are varied depending on substrates and existence of reactive gases.

Frederic Leroy, CNRS, France, presented his study of the self-organized growth of cobalt nanostructures on a silver thin film on a crystalline substrate. Data simulations performed in the distorted wave Born approximation framework demonstrate that the Co clusters grow above the dislocation crossing lines. **Rachel Segalman**, UC Berkeley, introduced her novel liquid crystalline rod-coil block copolymer, which has a lamellar morphology. She presented its phase diagram as a function of block ratio and temperature; grazing incident SAXS in conjunction with atomic force microscopy techniques were used. To conclude, **Young-Shin Jun**, UC Berkeley, demonstrated potentials of SAS techniques on environmental sciences. Simultaneous SAXS and GISAXS measurements enabled her to distinguish nucleation and growth behaviors of nanoparticles on a mineral surface from those in a bulk aqueous solution.

Byeongdu Lee

The technique of USAXS imaging and its theoretical basis was the topic of a talk by **Fan Zhang**, APS, Argonne. This technique combines USAXS with imaging, bridging the two to make a powerful tool for the characterization of scatterers in USAXS range and even larger. Finally, **V. Siva Kumar**, Georgia Inst. Tech., described his studies of precipitation. SAXS techniques are commonly used for these studies, but in this work it was clearly shown how important it is to extend the measured size range to the ultra small angle scattering region in order to understand the processes in these complex materials.

There was one poster related to this session, TP190, by **Trevor Willey** et al: *Small Angle X-ray Scattering from Transition Metal Oxide Aerogels*, which reviewed applications of USAXS to characterize the structure of these unique materials.

Jan Ilavsky and Kenneth Littrell

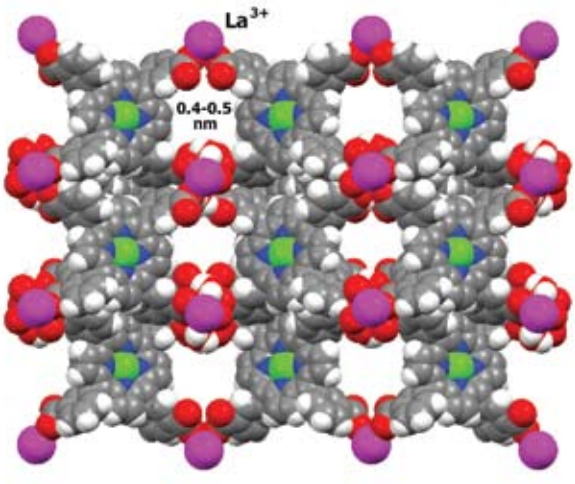
From left: David Rae, Richard Ibberson, Michelle Smith, Alberto Albinati, Michael Galella, Chick Wilson, Marilyn Olmstead, Larry Falvello, Israel Goldberg.

10.01 Important Science from Small Molecule Crystallography

At the behest of ACA president **Alan Pinkerton**, this symposium, which emphasized the importance of small molecule crystallography to science, was dedicated to the memory of **F. A. Cotton**. The depth and breadth of the research presented to a large audience provided a fitting memorial to Cotton, whose contributions to chemistry would in large part not have been possible without crystallography.

The first speaker, **Michelle Smith**, Kansas State, talked about the synthesis and characterization of ternary co-crystallants. There has been a renewal of interest in these compounds recently, especially by the pharmaceuticals industry. Michelle presented her logical approach to creating a ternary co-crystallized compound using a mixture of theoretical potential calculations and synthetic chemistry. **Marilyn Olmstead**, UC Davis, then described her studies of the *in situ* photolysis of azide from a variety of chromium complexes. This led to crystal to crystal transitions that were followed crystallographically. She spoke of the inherent problems with such experiments as well as the surprising result of a recrystallization on the microscope.

Israel Goldberg, Tel-Aviv U., described the use of porphyrins to create supramolecular cages and structures, with a view towards hydrogen storage.



From Israel Goldberg: space-filling view of the porous three-dimensional coordination polymer composed of tetra(m-carboxyphenyl) metalloporphyrin and lanthanide bridging ions down the 0.4-0.5 nm wide channels which propagate parallel to the c-axis of the crystal (see compound 1 in Inorg. Chem. (2007), 46, 5544-5554)..

Lanthanides were used in the chemistry as bridging atoms to alter the geometry of the pores within the lattice.

Chick Wilson, U.Glasgow, in speaking about his use of high-throughput neutron diffraction techniques, treated the audience to a lively discussion of his efforts to produce both variable temperature and pressure studies of small molecules. He focused particularly on the location of hydrogen-bonded atoms within these structures.

Alberto Albinati, U. Milan, who also used neutron difffraction techniques, discussed the coordination chemistry of hydrogen and the differences between solution and solid state compounds. He also used the complementary method of Pulsed Gradient Spin Echo (PGSE) NMR. **Richard Ibberson**, ISIS, described their state-of-the-art high-resolution powder diffractometer (HRPD) instrument and discussed the combined use of high-resolution neutron powder diffraction and single-crystal x-ray diffraction in characterizing the phase changes of cyclohexene. **Michael Galella**, Briston-Myers Squibb, gave an interesting talk about his characterization of a wide variety of water hyperacid compounds, proving that there is potential for a large number of $H_{2n+1}O_n$ cations. **David Rae**, Australian Nat'l U., emphasized the need to rationalize and describe structures more accurately. His discussed a methodology for the conceptual deconstruction of a complex (*i.e.*, "difficult") structure into components, which need not be identical, related by refinable twin and disorder relationships.

The afternoon session began with **Hamilton Napolitano**, UEG, Brazil, describing chalcone compounds and their relevance to the pharmaceutical industry. Continuing the neutron diffraction theme, **Paula Piccoli**, Argonne, discussed a series of exciting results, including bridging linear hydride complexes and unprecedented oxo-complexes of platinum and gold. **Joel Miller**, U.Utah, added a little local flavor for the session, with his discussion of the chemical and magnetic properties of a variety of cyanide containing complexes, including the very well known Prussian Blue. Remarkably, one of the compounds he studied has what can convincingly be called bonding interactions between carbon atoms at very long distances from each other. **Xiaoping Wang**, U.North Texas, bought the focus of the session back to F. A. Cotton with a presentation on Cotton's contributions to chemistry that could not have been achieved without crystallography.

Larry Falvello, U. Zaragosa, Spain, gave a well-received retrospective of the contributions that F.A. Cotton made to chemistry from his early years through to the modern day.

From left: Xiaoping Wang, Paula Piccoli, Alan Pinkerton, Larry Falvello, Carlos Murillo, Hamilton Napolitano, Lee Daniels, Joel Miller, Allen Oliver.

10.01 Important Science from Small Molecule Crystallography, cont'd.

Carlos Murillo, Texas A.& M., demonstrated that electronic structure can be obtained through variable temperature crystallography via bond distance measurements. **Lee Daniels**, Rigaku, commented on the need for charge density studies and advised care when undertaking such studies. In an historical note, Lee mentioned that the company formerly known as Molecular Structure Corporation (now Rigaku Americas), which brought Rigaku single-crystal diffractometers to North America, was founded three decades ago by young entrepreneurs who had studied chemical crystallography in Albert Cotton's research group. The final speaker, **Alan Pinkerton**, U.Toledo, also emphasized the challenges that one must overcome with charge density studies. and related an anecdote about Al Cotton that can be applied in research: Cotton observed while dining with Alan once that the amount of flavor in a strawberry is inversely proportional to it size.

Larry Falvello and Allen Oliver

Photo by Victor Young.

From left: Xiaoping Wang, Gary Enright, Ton Spek, Rob Hooft, Paula Piccoli, Phillip Fanwick, Larry Falvello, Victor Young.

10.02 Tricks of the Trade: Interpretation of Structural Results

Phil Fanwick, Purdue, led with the provacative presentation *Is Small Molecule Crystallography Still Science?* that explored comments from journal referees regarding the positional refinement of hydrogen atoms in a small organic molecule, namely, that the structural parameters of the hydrogen atoms were not reasonable. Through the use of scientific reasoning and a judicious search of the Cambridge Structural Database for similar neutron determined structures, he was able to show that his refinement of hydrogen atoms in the x-ray structure was valid and that the resulting parameters were in line with the analogous neutron structures.

Larry Falvello, U. Zaragosa, Spain, described *The Correct Use of Incorrect Space Groups and Unit Cells* focusing on using a subgroup of the correct space group to solve a difficult structure by identifying those symmetry elements that give questionable results and then using the highest order subgroup that does not possess those elements; it can then be factored into the correct space group. His second example was of a flexible coordination compound that undergoes a second-order phase transition upon being cooled (Cmcm at low temperature). Variable temperature x-ray diffraction and analysis of distortion parameters predicted that the temperature at which the molecule was undistorted was ~ 314°K (Fmmm). The 298ºK x-ray structure, barely distorted from the higher temperature phase, was not able to be solved in Cmcm and was therefore solved in the incorrect Fmmm, although distortion in the anisotropic displacement parameters is evident at this temperature.

Victor Young, U. MN, gave a presentation on the refinement of non-merohedral twins. In the variable temperature study of a twinned crystal of 2,2,3,3,4,4-hexafluoropentadiol, a phase change between 298°and 173°K revealed a new unit cell but similar twin laws, related by rotation about *a*. The packing of the unit cell indicated a pseudoglide in which the layers of molecules slip over each other in accordion fashion. Solutions for

cont'd. next page

10.02 Tricks of the Trade: Interpretation of Structural Results, cont'd.

twin problems can include moving the detector back; using Cu radiation to improve the spatial resolution of the twinned reflections; or adjusting the temperature. There are many programs now available to make HKL files from twinned data.

Ton Spek, U. Utrecht, spoke on some of the many features of PLATON, a most useful tool for structure validation. The ADDSYM (checks for higher symmetry in a structure), TwinRotMat (automatic twinning analysis), SOLV (analysis of solvent accessible voids), and SQUEEZE (back-Fourier transformation of disordered solvent, which outputs a "solvent-free" HKL file for further refinement) features were all highlighted.

Xiaoping Wang, U. North Texas, presented his careful examination of the $Ta(NMe_2)_5$ structure, which has molecular C_2 symmetry. Originally solved in the incorrect space group Cmcm. At lower tempature symmetry-imposed disorder was discovered. Subgroups Pbcn (molecular symmetry C_2) and Pnma (C_{2v}) were possibilities for the correct space group; however when the tolerance for indexing the diffraction peaks was relaxed, the software found the correct Pbcn space group. The structure was then refined with no symmetry imposed disorder.

In a complex analysis of a composite crystal with distinct structural domains, **Gary Enright**, NRC, Canada, used both ^{129}Xe NMR and x-ray diffraction to characterize the loading of Xe into *p*-tertbutylcalix[4]arene (tBC). At various degrees of Xe loading into the host, two distinct guest sites are populated. The Xe-Xe distance increases with loading, but the transition is not continuous and loading of the guest leads to a structural rearrangement of the molecules within the crystal. Additional racemic twinning is found at higher pressures of Xe, complicating the analysis. This is a great example of single crystal phase transformation in which more than one phase can be seen in distinct domains.

Rob Hooft, Bruker AXS, then demonstrated the use of Bayesian statistics in determining the absolute structure of small pharmaceutical molecules (light atom structures) using Mo radiation. By carefully measuring Bijvoet pairs and assigning weights to each difference, the probability theory contained in PLATON gives a measure of whether the structure is of one handedness or the other. The statistical uncertainty from this method has been shown to be smaller than that found with the more conventional Flack parameter, and is a promising technique in establishing the absolute configuration of light atom structures using Mo radiation.

We hope to have some of these presentations available for public download at **www.pns.anl.gov/instruments/scd/subscd/scd.shtml.**

Paula Piccoli

From left: Silas Blackstock, Miguel Garcia-Garibay, Tara Burchell, Kenneth Doxsee, Jesus Valdés-Martinez, Radu Custelcean, Bruce Foxman, Alicia Beatty, Len Barbour, Greg Hogan, and Chister Aakeröy.

10.03 Supramolecular Chemistry

Speakers in this all-day session addressed a wide range of topics directed at the general theme of decoding the architectures and utility of supramolecular assemblies. This session also sponsored a student poster competition with awards given to **Volodymyr Vreshch**, **SP209**, **Dejan-Krešimir Bučar**, **TP251**, and **Aribin Rajbanshi**, **SP207**.

Bruce Foxman, Brandeis, began with an energetic discussion of the solid-state reactivity of metal carboxylates, with insights about the structural features of materials that undergo regio and stereo controlled reaction processes. **Radu Custelcean**, ORNL, described the use of competitive crystallization of metal-organic frameworks as a method for the separation of anionic species. His many examples showed inclusion of these anions often followed a shape/size selection process. **Christer Aakeröy**, Kansas State U., gave an engaging presentation on the design strategy and preparation of ternary co-crystalline materials that was well received. Christer showed how his simple (yet elegant and effective) uses of hydrogen bond connections aided in the construction of these three-component systems. **Kenneth Doxsee**, U.Oregon, showed how salt metathesis reactions provide a versatile synthetic route to a wide variety of solid-state materials. Since reaction crystallizations often include solvation and chelation processes, this method of crystal growth affects the morphology and phase of crystalline solids. **Tara Burchell**, NRC, Canada, described the crystal chemistry of the tripeptide L-Leucyl-L-Leucyl-L-Leucine. By altering the crystallization conditions, this peptide was shown to adopt a variety of conformations and crystal packing motifs with solvent and small organic guest molecules. The topic of intercalation of hydrogen bonded solids was presented by **Alicia Beatty**, Mississippi State U. Her work on both inorganic

and organic "clay mimics" showed how crystallographic and TGA data relate closely to the observed inclusion behavior.

The afternoon session began with an elegant talk by **Miguel Garcia-Garibay**, UCLA. He demonstrated that his carefully designed amphidynamic crystals (materials with functions controlled by internal molecular motion) are capable of behaving like molecular gyroscopes. The many examples presented showed how the dynamic properties depend on the structure. **Jesus Valdés-Martínez**, U.N.Autónoma de México, then examined the structures of 4-pyridinealdoxime organic hybrid materials and the role of pendant alkyl groups in the alignment of the oxime…oxime interactions. Both **John MacDonald**, Worchester Polytechnic, and **Len Barbour**, U.Stellenbosch, South Africa, presented their work on designing and constructing porous organic-hybrid materials. Their discussions gave excellent insights into fundamental aspects of molecular recognition and new developments for the preparation of practically useful porous materials. **Greg Hogan**, Mississippi State U., (an **Etter Student Lecture Awardee**) described his work on layered materials created from metal-containing dicarboxylic acid organic amines. **Silas Blackstock**, U. Alabama, gave important crystallographic perspectives on organic polar materials. His presentation described a set of aryl diamines which assemble into polar motifs. By altering various regions of the molecular structure, he was able to show the dependency of specific chemical features to the polar alignment of the building-blocks.

Kraig Wheeler, left, presenting Greg Hogan with the Etter Student Lecture Award.

Kraig Wheeler

(Photos courtesy of Kraig Wheeler.)

From left: Janaina Ferreira, Michael Sawaya, Bill Ojala, Francesca Fabbiani, Christine Beavers, Maxime Siegler, Allen Oliver.

10.04 Cool Structures

The Cool Structures session began with a talk by **Maxime Siegler**, U. Kentucky, discussing some interesting "trapped" transitional phase change structures of 15-crown-5 complexes. **Michael Sawaya**, UCLA, followed with a presentation on the structure of fibril-like compounds, their packing and the implications of these compounds in amyloid-based diseases. **Janaina Ferraira**, Universidade de São Paulo, Brazil, gave a talk about the structure and inter-molecular bonding found in a pair of related copper azido complexes formed in the same reaction. **William Ojala**, U. St. Thomas, presented both his successes and his not-so-successful attempts to find and co-crystallize "bridge-flipped" benzanilide and hydrozone compounds. **Christine Beavers**, UC Davis, gave an interesting talk on the effects of aurophilicity, as demonstrated in her complex. One compound exhibited 3 gold species, monomer, dimer and trimer. In the concluding talk **Francesca Fabbiani**, ISIS, UK, demonstrated and classified the polymorphism of the molecule carbamazepine.

Allen Oliver

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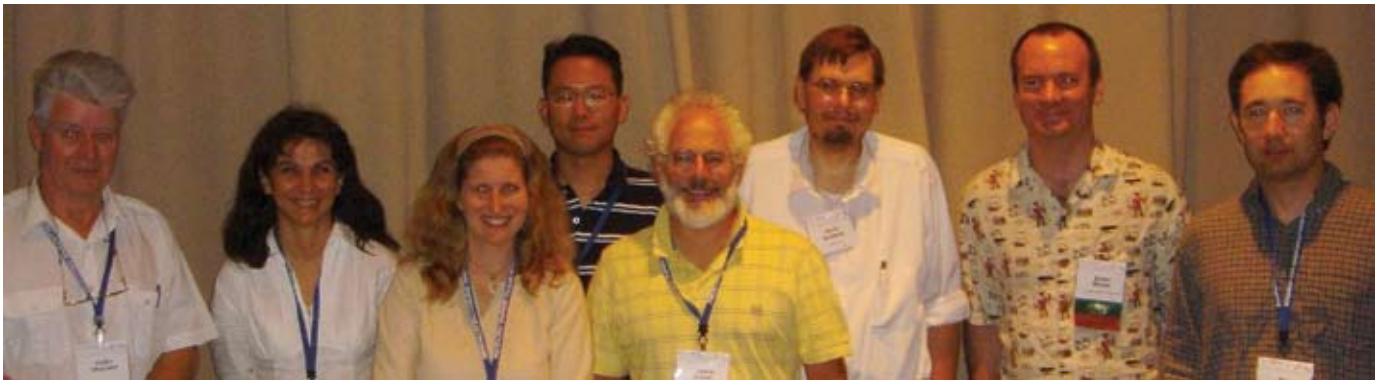
From left: Bobby Huether, Peter Horanyi, Cora Lind, Jenny Glusker, Jasmine Young.

12.01: FLYS – Fun Lectures for Young Scientists

The FLYS session began with a seminar by the Etter Award winner **Cora Lind**, U. Toledo. She emphasized the importance of the connections made throughout her early career and how they helped her. **Jasmine Young**, Rutgers, an annotator from the PDB, gave us 5 easy steps that make it easy to deposit a structure. **Jenny Glusker**, Fox Chase Cancer Center, presented a very interesting history lesson about crystallography, from the days of predominately small molecules to larger macromolecules, in the process singing a little rhyme about Lindo Patterson. **Peter Horanyi**, U. Virginia, gave an informative talk on how to get a post doc. Peter has made his slides available for everyone, they have been posted on the ACA website.

Bobby Huether



From left: Andre Mitschler, Magdalena Ivanova, Aina Cohen, Chai Un Kim, Steve Ginell, Dave Bushnell, James Holton, Max Nanao. Photo courtesy of Aina Cohen.

13.01: Advances in Data Collection

This session, co-sponsored by the Young Scientist SIG and the Synchrotron Radiation SIG, focused on new techniques in sample preparation, data collection, and data processing. The emphasis was on education with the goal of training others to try these new methods and learn from the success of others in challenging areas of research. **Dave Bushnell**, Stanford, began by sharing many lessons learned by the Kornberg group in over a decade of structural investigation of RNA polymerase II, a half megaDalton complex comprised of 12 subunits and more than 4500 amino acids. The group overcame the many challenges of studying very large proteins complexes and their efforts ultimmately let to the award of the Nobel Prize in chemistry in 2006 (see p. 34). **Andre Mitschler**, U. Strasbourg, France, followed with a presentation on the very high resolution structure of human aldose reductase. A joint refinement of neutron and x-ray diffraction data enhanced the visibility of a mobile catalytic proton demonstrating the benefits of combining these techniques for protein crystals that diffract to < 1 Å resolution. **Magdalena Ivanova**, UCLA, described structural studies of amyloid-like segments that form a dry tightly self-complementing 'steric zipper' structure which may be similar those in amyloid plaques associated with diseases such as Alzheimer's, Parkinson's, and prion diseases. Because the segments tend to form microcrystals which do not survive long in the x-ray beam, diffraction from many crystals was combined to form a complete dataset. **Max Nanao**, Exelixis, discussed the use of UV-induced structural changes to phase macromolecular structures. The advantage of UV radiation is that the damage is specific and UV does not induce as many changes as x-ray radiation. Examples were presented and the location of the UV damage was shown. **James Holton**, LBNL, followed with a very stimulating talk on how structural biologists can improve their efficiency and success in structure determination by doing the data collection process correctly. The take home message is to avoid or minimize radiation damage. **Chae Un Kim**, Cornell, discussed recent advances in the use of high pressures while cryo cooling crystals. It was shown that macromolecular crystals in native mother liquor without the use of cryoprotectants could be flash frozen at high pressures while in a capillary. A pertinent example was the structure of thaumatin, which was solved by sulphur SAD phasing.

Aina E. Cohen and Stephan L. Ginell

13.02 Detectors

Talks in this session ranged from new detector hardware designs and their potential applications to new methods for correcting and improving crystallographic data from detectors already in widespread use (mosaic CCD detectors). **Masaki Yamamoto**, RIKEN/ SPRING-8, discussed a solid state flat-panel design of a large area detector developed in Japan and tested at a SPRING-8 beam line, which at this stage produces images that would be useful for continuous data collection. **Ed Westbrook**, Molecular Biology Consortium, discussed a silicon Pixel Array Detector (PAD) design in the prototype stage that features a high signal per x-ray (to achieve single photon counting resolution in an analog device) and uses continuous read out. **Mark Tate**, Cornell, gave a survey of the PAD designs from the Swiss Light Source (a digital PAD), Cornell (an analog PAD design), and an ADSC-Cornell design (a mixed mode analog and digital PAD). An example of a time-resolved experiment using the analog PAD of a diesel engine fuel injection system demonstrated the fast time resolution of this detector.

Andy Arvai, Scripps, gave a talk outlining the problems for crystallographic data near the corners of mosaic or array CCD detectors with examples of under-measured data near corners. He described

From left, standing: Chris Nielsen, Thomas Earnest, Mark Tate, Ed Westbrook; sitting: Gerard Bricogne, Masaki Yamamoto, Andy Arvai.

how the problem derives from the change in point spread behavior in the tails of reflections from the center of the CCD module to the corner. He proposed a correction method to be applied to integrated data as a function of position on the detector. **Gerard Bricogne**, Global Phasing, UK, presented some preliminary results from his group concerning the corner correction problem. He discussed characterizing the point spread variation using statistical fluctuations in flood fields and analysis of calibration masks. The goal is to derive information needed for the corner correction using calibration data that all manufacturers have for every detector as opposed to a correction based on experimental data. This work is still in the preliminary stage.

Thomas Earnest and Christopher Nielsen

From left: William Heller, Lin Yang, Günter Grossmann, Susan Krueger, Jan Lipfert, Jill Trewhella, Tracy Nixon, Joanna Krueger, Thomas Weiss.

13.03 Biomolecular Assemblies and Biomembranes

This session, co-sponsored by the small angle scattering SIG and the biological macromolecules SIG, focused on the application of non-crystalline small angle scattering to biological macromolecular assemblies and biomembranes.

Tracy Nixon, Penn State, presented a detailed structural model of the assembly and mechanism of the AAA+ ATPase, a molecular motor that regulates the transcription of genes by the σ54-form of bacterial RNA polymerase. The model, based on a combination of solution scattering data, electron microscopy and atomic models of isolated subdomains, explains in fascinating detail how the ATPase is assembled and the RNA polymerase is released to begin transcription.

Lin Yang, Brookhaven National Lab, showed how grazing incident scattering at the lipid-water interface can be applied to monitor the two-dimensional ordering of proteins and viruses. Using a biotin-streptavidin link between lipid molecules at the air-water interface and the protein/virus particles in the water subphase, the particles are trapped at the lipid water interface yet keep their lateral mobility. He showed that by tuning the inter-particle interaction through additives in the water subphase, the formation of well ordered two-dimensional structures can be initiated.

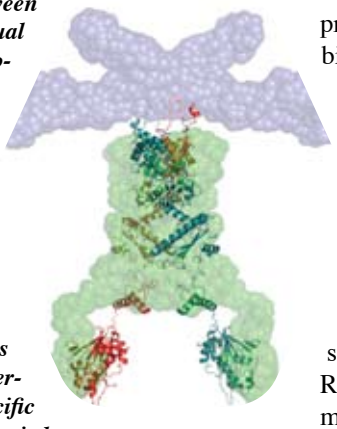
Susan Krueger, NIST, NCNR, reported in her presentation on the recent efforts at the NCNR to develop new software tools and methods specifically aimed towards the modeling of intrinsically disordered proteins. She illustrated these methods in two studies of two nucleic acid binding proteins in solution: HIV-1 Gag and the mini-chromosone maintenance complex. The inher-

cont'd, next page

13.02: Detectors cont'd.

ent unstructured nature of these proteins resulted in scattering data from an ensemble of structures, and the structural modeling performed focused on identifying a suitable population of structures with calculated intensity profiles that best reproduced the measured data.

Günter Grossmann, Daresbury Lab., UK, set the stage using examples of different proteins and protein complexes to show how recently available enhanced data analysis and interpretation procedures can produce reliable low-resolution structures, thereby allowing improved insight into questions of biological interest. He pointed out that in some cases differences between solution scattering models and crystal-structures are likely due to distortions of the protein conformation by the packing forces inside the crystal which are absent in solution.



From Gunter Grossman: an encounter between multi-domain chaperone molecules. Individual molecular conformations of the heat shock protein 90 (Hsp90, green) and Hsp90 organizing protein (Hop, blue) have been restored from small angle x-ray scattering (SAXS) data and are displayed as arrays of spheres. A two-fold symmetry constraint was applied owing to the dimeric nature of the two proteins. Crystallographic information of Hsp90 domains has been exploited to model the nucleotide-free state of the chaperone in harmony with SAXS data. The graphic shows a possible docking situation during which C-terminal Hsp90 segments are recognized by specific binding regions of Hop. Experiments were carried out at the Daresbury SRS, UK, in collaboration with S.E. Jackson and S.C. Onuoha, Cambridge U. Chem. Lab., UK.

Jan, at left, receiving the award from session chair Thomas Weiss.

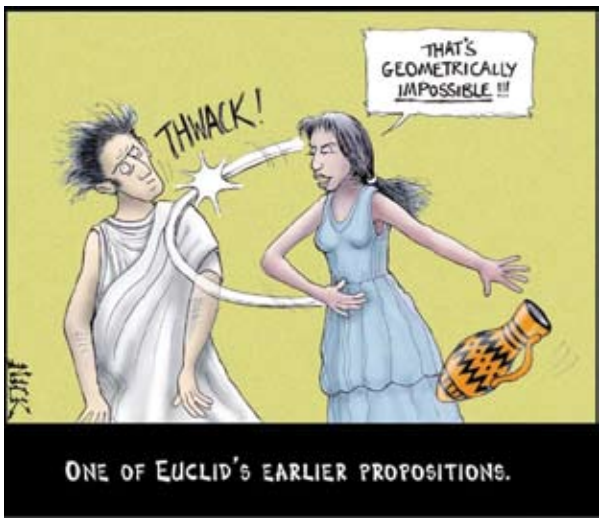
Jan Lipfert, Stanford, who received an **Etter Student Lecturer Award** for his presentation, reported on his work using solution x-ray scattering on protein detergent complexes (PDC) of the integral membrane protein TM0026. He showed that it is possible to separate the "empty" micelle scattering from the signal of the PDC and that this is an aid to structure elucidation. Using additional data from NMR and EPR spectroscopy he was able to construct intermediate resolution models of the PDC. He presented evidence that the TM0026 adopts different conformations depending on the chain length of the detergent, suggesting that there is an optimal size of the micelle for membrane protein studies.

Jill Trewella, U. Sydney,explained how the combination of x-ray solution scattering, homology modeling and neutron contrast variation can be used to unambiguously determine three dimensional arrangements of complex protein assemblies. She presented the structure of the neuroligins/neurexin complex within the synaptic cleft. Because mutations of the neuroligin and neurexin genes appear to be linked to autism and mental retardation, the results presented provide a structural framework for understanding such developmental disorders.

Joanna Krueger, UNC Charlotte, gave an overview of the fundamentals of solution small-angle scattering for studying protein complexes. She also presented exciting results from her group's studies of the calcium activation of gelsolin, a protein involved in regulation of the cytoskeleton. Upon binding calcium, the 6-domain gelsolin adopts a more open conformation that was previously proposed to expose the three actin-binding domains of the molecule. Structural modeling suggested that reorientation of two domains of gelsolin are required upon actin binding.

William Heller, ORNL, described the Center for Structural Molecular Biology at ORNL, a user facility for neutron scattering from biological systems. The centerpeice of the effort is a new small-angle neutron scattering (SANS) instrument at the High Flux Isotope Reactor that recently entered commisioning. The new instrument is complemented by the Bio-Deuteration Laboratory which produces isotopically labeled proteins for neutron scattering studies. The new SANS instrument together with other neutron scattering instruments at ORNL such as the Liquids Reflectometer and the Macromolecular Neutron Diffractometer (MaNDi) at the Spallation Neutron Source will make the facility attractive to users.

Thomas Weiss and William Heller



By *Nick D. Kim, U. Waikato, New Zealand.*
See nearingzero.net/res.html.

13.04: Time and Field Dependent Responses in Scattering Experiments

From left, standing: Claudia Rawn, Jonathan Hanson, Vitalij Pecharsky, Ashfia Huq, Volker Urban, sitting: Wim Pyckhout-Hintzen, Charles Dewhurst, Thomas G. Mason.

This session, co-organized by the Small Angle Scattering and Materials SIGs, covered a broad range of experimental research, in which response to external fields as well as evolution over time is essential.

Charles Dewhurst, Institute Laue-Langevin, France, commenced with an impressive overview of current research on magnetic flux line or vortex lattices (VL) in type II superconductors revealed by magnetic small angle neutron diffraction. These materials include high-temperature superconductors, multi-band, heavy-fermion and unconventional materials, and non-local superconductors, as well as 'classic' materials such as Nb. Examples included non-magnetic borocarbide materials, such as [Y or Lu]Ni_2B_2C and heavy-fermion $CeCoIn_5$, where nonlocal effects and Fermi surface anisotropy determine a range of VL structures and phase transitions from nearly hexagonal at low fields to distorted rhombic and square lattices at higher fields. The first imaging results of VL under applied current perpendicular and vertical to the applied field were also discussed.

Wim Pyckhout-Hintzen, Forschungszentrum Jülich, Germany, changed the topic from magnetic fields to mechanical shear stress fields in the hierarchical relaxation of non-linearly stretched, branched polymers. In this research investigations typically aim at coupling rheology and neutron scattering and at providing a toolbox for the prediction of the processing properties of such new soft composites. Wim highlighted recent progress made through advances in tube model theory, availability of model polymers with H-shaped and hyperbranched architecture as well as development of advanced random phase theory to account for elastic fluctuations and inhomogeneities.

Thomas Mason, UCLA, then took the combined approach, Rheological Small Angle Neutron Scattering (Rheo-SANS) into a different area of materials: the structure of nanoscale droplets in jammed networks of attractive nanoemulsions. Application of high shear stress leads to unmistakable changes in the structure. The scattering experiment revealed shear-induced de-gelling of the attractively jammed networks because of a limited degree of disaggregation of nanodroplets.

Jonathan Hanson, BNL, continued the session by discussing Time-Resolved X-Ray Diffraction (TR-XRD) for characterizing catalysts and active sites. Hanson described the NSLS beamline X7B where subminute TR-XRD experiments can be conducted under a variety of temperature and pressure conditions as well as gas environments. The TR-XRD studies are used to determine structural details, phase composition, kinetics of transformations, and intermediate phases. Examples of studies on zeolites and various oxide catalysts were presented.

Vitalij Pecharsky, Ames Lab & Iowa State U., described a laboratory experimental set-up with a rotating anode powder diffractometer coupled with a close cycled He cooled refrigerator and a split-coil superconducting magnet. With this set-up, Rietveld quality data can be collected at temperatures ranging from 5 - 315°K and magnetic fields up to 4 T. Data sufficient to quantify phase fractions and changes in lattice parameters can be collected in 20 minutes or less. High quality data necessary for detailed individual atomic parameters can be collected in a few hours. This instrument can be used to study field-induced structural changes.

Ashfia Huq, ORNL, ended the session by discussing time-resolved neutron diffraction studies used to study the structure of lithium imide. *In-situ* data were collected on the cubic lithium imide at 250ºC during hydrogenation and dehydrogenation. The data were then used to understand the disorder of the hydrogen positions in the structure.

Volker Urban, Claudia Rawn, & Lionel Porcar

Photo of the SLC Convention Center by Peter Müller.

From left: Axel Brunger, Yizhi Tao, Winfried Weissenhorn, Peter Kwong, Theodore Jardetzky.

13.05: Structural Mechanisms of Infectious Diseases

Jeffrey Kieft, U. Colorado, addressed the mechanism of virus-mediated translation initiation. For normal cellular RNA transcripts, ribosomal translation initiation is dependent on a well-defined cap structure. Cap-independent transcription was first described for viral RNAs and led to the discovery of internal ribosome entry sites (IRESes). The viral IRESes are structured RNA sequences that replace the function of the mRNA cap. Kieft described the crystal structures of two distinct domains of a viral intergenic region (IGR) IRES. The larger IRES domain binds to the 40S subunit leading to the recruitment of the 60S subunit, and is probably accompanied by conformational changes within the IRES induced by ribosome binding. The structure of the smaller, IRES P site domain was also presented; the P site domain forms a pseudoknot which mimics the codon:anticodon interactions that occur naturally during translation. The crystal structures of the two RNA domains were fit into low resolution EM maps, providing a detailed model of how viruses can bypass the normal requirements for mRNA translation.

Jane Tao, Rice, tackled the issue of genomic RNA packaging in influenza viruses. Influenza pandemics have had tremendous impact on society, as exemplified by the drop in US life expectancy that accompanied the 1918 influenza pandemic and the current fears about a spread of the deadly "bird" flu to humans. Influenza virus consists of 8 separate RNA segments that are packaged together with the viral nucleoprotein, as well as other viral proteins, into a compact helical ribonucleoprotein complex. Tao described the purification of the influenza NP protein, which forms higher order oligomers on its own. By testing a variety of influenza strains and treating NP with proteases, crystals of NP were obtained containing a trimer of the protein. Two interfaces contribute to the observed NP trimer: it is not 3-fold symmetric, but a 'tail" loop plays a major role in the interactions, as mutations in this region result in a monomeric NP. The structural results suggest how NP may bind to RNA and assemble, with some oligomeric flexibility, into the final helical RNP. Tao suggested that the oligomerization regions of NP would be attractive targets for novel anti-influenza therapeutics.

Winfried Weissenhorn, EMBL, continued with the theme of viral RNA genome compaction, using rabiesvirus N protein as a model system. When the nucleoprotein of rabiesvirus is expressed it spontaneously assembles with RNAs into oligomeric coils and rings reminiscent of the viral RNP structures. N rings containing 9, 10, 11, 12 and 13 subunits could be separated by large scale native gel electrophoresis and crystallized. The structure of the NP:RNA complex reveals RNA binding between two domains, mostly contacting the N-terminal region of NP. Domain swapping between protomers ties together the oligomer. Variability in interactions potentially provides adaptability of the RNP to form its final packaged helical structure. The bilobed structure of the rabiesvirus NP and its interaction with RNA may be conserved in other viruses, as EM and crystallographic studies of paramyxoviruses, filoviruses and bornaviruses suggest direct parallels. The structure likely represents a closed form, which must open up to allow polymerase access to the viral genome. Small molecules directed at stabilizing this closed form might provide novel antiviral agents.

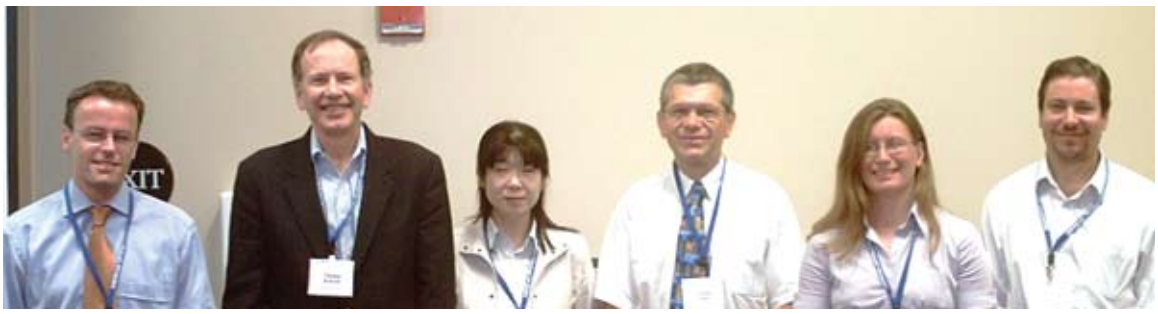
Axel Brunger, Stanford, HHMI, presented structural results that have led to an improved molecular level understanding of how botulinum neurotoxin (BoNT) binds to its protein receptor and ultimately cleaves SNARE proteins that are essential components of the synaptic vesicle fusion machinery critical for neurotransmission. Receptor binding is mediated by induced helix formation in the luminal domain of the receptor and docking of this helix to a saddle-shaped crevice on a distal tip of BoNT. The proteolytic domain of BoNT is a zinc-dependent endopeptidase with similarities to thermolysin. Mutations at two active site residues yielded an inactive BoNT proteolytic domain that was co-crystallized bound to a SNARE protein substrate. In contrast to many proteases where substrate recognition is mediated by a small number of key localized interactions, structural and kinetic data for BoNT/SNARE reveal a large number of exosites that are involved in substrate recognition.

Ted Jardetzky, Northwestern, reported results from his studies of molecular interactions that mediate entry of enveloped viruses into target cells. In paramyxoviruses, two viral glycoproteins, an attachment protein and a fusion protein, drive the fusion of viral and cellular membranes. Structures were reported for the parainfluenza virus 5 (SV5) hemagglutinin/neuraminidase (HN) protein and for fusion (F) proteins from human parainfluenza virus 3 (hPIV3) and SV5. The hPIV3 F protein crystallizes in a post-fusion conformation while the structure of the SV5 F protein shows it to be in a pre-fusion conformation. Comparison of these two F proteins indicates major conformational differences involving both secondary and tertiary structure between the pre- and post-fusion states. The two F protein structures represent discrete folding intermediates in the overall conformational transitions leading to membrane fusion. From a study of these structures, an elegant overall model for F-mediated membrane fusion was proposed.

A major frustration surrounding efforts to develop an effective vaccine against HIV-1 has been that features of the viral envelope spike (composed of three copies of gp120) allow it to evade antibody-

mediated neutralization. Viral entry is facilitated by binding of gp120 to cell surface CD4. **Peter Kwong**, NAID/NIH, described a stabilized gp120 construct designed to retain a CD4-bound conformation even in the absence of CD4. His laboratory then used one of the few known broadly neutralizing HIV-1 antibodies (b12) to form a complex with the stabilized gp120 molecule. The complex was crystallized and its structure determined at 2.3 Å resolution. Thermodynamic characterization of the interaction between stabilized gp120 and CD4 suggested that the initial contact surface recognized by CD4 exists in the glycoprotein prior to any CD4 induced conformational changes. It turns out that antibody b12 binds to the same constitutively exposed surface recognized initially by CD4 and uses this functionally conserved contact site to neutralize diverse primary isolates of HIV-1. This structural information could be useful in the design of an effective HIV-1 vaccine.

Theodore Jardetsky and Dave Matthews



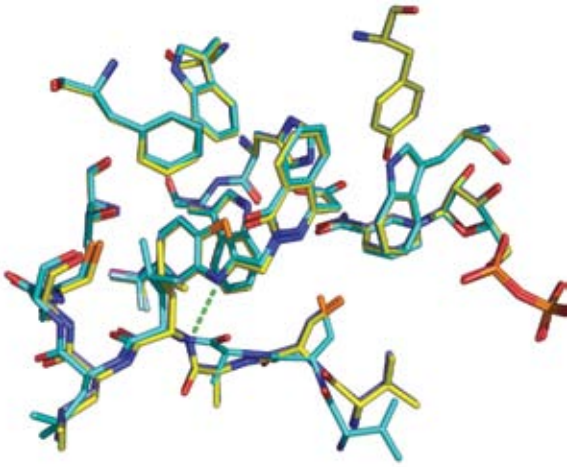
From left: Foldeo Mulder, Tom Koetzle, Yumiko Nakamura, Jacques Huot, Ewa Rönnebro, Anibal Ramirez-Cuesta.

13.06: Energy Storage and Conversion

This session offered a broad view of the synthesis and characterization of hydrogen storage materials. Neutron diffraction techniques were particularly well represented. **Anibal Ramirez-Cuesta**, ISIS, UK, showed some applications of Inelastic Neutron Scattering (INS) for probing hydrogen vibration levels and also discussed the merits of local density approximation and generalized gradient approximation in density functional theory for explaining the INS spectra of hydride materials. **Foldeo Mulder**, FAME R3, Switzerland, talked about the effects of nanostructure on the behavior of hydrogen storage materials and lithium ion battery electrodes. He demonstrated the use of neutron diffraction for probing phase transformations during hydrogenation and lithium diffusion. The new class of hydrogen storage materials, ammonia borane (H_3NBH_3), was the topic chosen by **Tom Koetzle**, Argonne. He presented the crystal structure of a pincer complex catalyst determined by single crystal neutron diffraction. A new metal hydride, the quaternary compound K_2LiAlH_6, prepared by a high pressure technique, was presented by **Ewa Rönnebro**, Sandia Nat'l Lab. The crystal structure of this new compound was investigated by x-ray synchrotron radiation. A new borohydride compound with high hydrogen storage capacity, $Ca(BH_4)_2$, was also presented. An *in-situ* neutron diffraction investigation of a more conventional alloy $LaNi_{5-a}M_aD_x$ (M = Al, Sn) was reported by **Yumiko Nakamura**, AIST, Japan. A detailed analysis of line broadening revealed that it is caused by anisotropic lattice strain.

Jacques Huot

Structure and Function Posters



From Andreas Heine: Superposition of three refined aldose reductase structures in complex with the inhibitor zopolrestat obtained by varying soaking and cocrystallization times. The structure obtained after 1 day of soaking (yellow) is virtually identical to the structure after 10 days of co-crystallization (blue). In contrast, after 3 or 6 days (cyan structure) of soaking, the previously observed hydrogen bond interaction is lost due to a peptide flip. (H.Steuber, M.Zentgraf, C.Gerlach, C.A.Sotriffer, A.Heine, G.Klebe (2006) J. Mol. Biol 363, 174-187.)

A poster by **Andreas Heine** et al, Philllips U.- Marburg, Germany, entitled *Crystallographic Pitfalls in Structure Based Drug Design*, **TP110** gave three examples where different crystallization or ligand soaking conditions revealed unexpected structural changes such as different binding modes for the same ligand, space group transitions, or additional metal binding sites.

Poster **TP114**, *From Macromolecular Crystal Structure to Reliable Electrostatic Interactions* by **Philip Coppens** et al, SUNY, Buffalo, showed the effects of using aspherical electron distributions to calculate electrostatic interaction energies that are better than those obtained using point-charge models.

Another interesting poster, **TP249**, *PriB-ssDNA Structure Suggests a Novel Single-stranded DNA Binding Mode* by **Chwan-Deng Hsiao** et al, Academia Sinica, Taiwan, showed a different mode of binding of single-stranded DNA than that found in other complexes with related ssDNA-binding proteins.

Ron Stenkamp and Vivian Cody

From left: Shilpa Sambashivan, Malcolm Capel, David Flot, Richard Gillilan, Ruslan Sanishvili, Meitian Wang, and Gerd Rosenbaum.

Photo courtesy of Richard Gillilan.

13.08: Microcrystals, Microbeams, and Multiple Crystals

Every crystallographer hopes for large, well-formed crystals, but in practice ideal conditions are rarely met. In fact, microcrystals (< 20 μm in diameter) are becoming more and more common as researchers investigate more challenging biological systems. As an introduction, **Gerd Rosenbaum**, APS, gave an overview, identifying 8 synchrotron beamlines worldwide capable of microcrystallography and predicting a doubling of this number given the construction now underway. Speakers addressed three main topics: x-ray optics, endstation instrumentation, and examples of the scientific advances made possible by microbeam technology.

Shilpa Sambashivan, Stanford, spoke about her work with David Eisenberg's group at UCLA, on fibril-forming peptides related to Alzheimer's Disease. Critical peptide segments from a wide variety of proteins associated with amyloid diseases have been identified which preserve the fibril-forming characteristic of the diseases, but also permit crystal formation. Because these peptides prefer to form fibrils, crystals tend to be very small (typically needles < 2 μm in diameter) and it is necessary to screen many samples to obtain adequate diffraction quality. Unusual techniques are also required in which crystals are mounted on glass fibers completely removed from solvent. Sambashivan collects data using (5 μm) microbeam facilities at ESRF ID13 (Christian Riekel) and at SLS X06SA (Emke Pohl). Now that more than 30 different peptide segments have been examined, a general picture of fibril formation is emerging which will shed light on numerous amyloid diseases.

Meitian Wang, (speaking on behalf of Clemens Schulze-Briese, SLS), described an international collaboration of groups working on naturally-occurring protein microcrystals with a biological function ***(see Coulibaly et al., (2007) Nature 446, pp 97-101)***. Insect cells infected with cytoplasmic polyhedrosis virus actually produce 2 μm crystals within the cell cytoplasm. These tightly-packed protein crystals (polyhedra) act as protective envelopes for infectious virus particles. Because of extreme resistance to degradation, *in vitro* crystallization has not been possible and, until now, polyhedra have been considered too small for single-crystal diffraction. Wang described using MicroMesh mounts (MiTeGen) to harvest crystals and remove excess solvent. Using an attenuated microbeam with a MD2 diffractometer at the SLS beamline X06SA, the protein structure was solved to 2.1 Å.

Ruslan Sanishvili, Argonne, combines focusing (70x20 μm) with a 10 μm aperture and scatter guard to obtain a low divergence "minibeam" at GM/CA-CAT (APS). While the data show excellent statistics, Sanishvili cautioned that minibeams should generally be used as a last resort and not as an alternative to growing good large crystals. Although large crystals in "standard" beams produce better data, microbeams can still be useful even for large samples. For example, refined mosaicities are significantly lower for micro-beams. Also, split spots and/or satellites can be better resolved. Sanishvili suggests that samples might be screened first with a minibeam in order to locate the best diffracting regions. Full data collection could then be made with a larger beam diameter. Preliminary design specifications were given for a dual collimator system that would make changing the beam diameter easier. **Malcolm Capel**, NE-CAT, APS, described an active feedback system implemented to compensate for beam motion down to 1 μm. For microcrystallography, a commercial MD2 setup with a retracting aperture assembly close to the sample is used. Beams typically require 20-50% attenuation. Capel discussed the case of a 16x16x140 micron crystal in which a full dataset was assembled by scanning the microbeam and then merging data from different parts of the crystal. In the future, autorastering software, in which the user specifies a scan path for the beam along the crystal, is expected to be important.

David Flot, EMBL-Grenoble, introduced ID23-2, a new dedicated protein microcrystallography beamline which is routinely capable of providing 7x5 μm diameter (FWHM) x-ray beams. At 45 meters from the source, it uses a single-bounce monochromator and a simplified version of the commercial MD2 microdiffractometer. Positional beam drift due to temperature variation has been measured at only 5 μm per day. Crystals as small as 5x5x5 μm have been observed. ESRF MX staff and the EMBL-Grenoble "instrumentation group" are working on UV-based crystal centering. Automatic collection of data on multiple crystals in one loop is also expected to be important in the future.

Richard Gillilan, MacCHESS, Cornell, ended the session by describing microcrystallography at Cornell's High-Energy Synchrotron Source (CHESS). X-ray beams 18 μm in diameter are produced with a unique single-bounce capillary optics system mounted close to the sample. Gillilan demonstrated how by running helium through a standard LN2 cryostat at 100°K and enclosing the sample, x-ray optic, and beamstop within the helium atmosphere, a three-fold factor of improvement in signal-to-noise could be observed in a test microcrystal comapared to a nitrogen atmosphere. Confirming similar observations by earlier speakers, because larger crystals are often inhomogeneous in quality, a judiciously-placed microbeam can sometimes yield significantly improved diffraction.

Richard Gillilan and Gerd Rosenbaum

From left:. Peter Müller, Bruce Foxman, Jörg Kärcher, Jenny Glusker and Henk Schenk. Some speakers are holding gadgets.

Photo by Peter Müller.

13.09: Teaching Gadgets and Educational Tools

This very well attended session was organized by **Peter Müller**, MIT, and focused on physical gadgets to teach crystallographic topics as well as computer based teaching approaches. Peter Müller began with *Are Teaching Gadgets Obsolete in Times of Computer Animations?* Not surprisingly, the answer to this question turned out to be ***no***. Peter dedicated his talk to Wally Cordes, the "Godfather of crystallographic teaching gadgets," and showed a large variety of teaching tools, both store bought and home made.

During her talk *Crystallographic Teaching Tools for Beginners*, Jenny Glusker, Fox Chase Center, also showed many different teaching gadgets, such as simple fabric samples from a hardware store as diffraction grids, a goniometer key stuck in a styrofoam cup pointed at a photograph of a diffraction pattern as a model of a diffractometer, a calcite crystal to demonstrate double refraction, and many others. Her main message was that the teacher should always encourage the student to appreciate the practical and three-dimensional aspects of crystallography. In his presentation *Walking the Reciprocal Space: Beyond Bragg & Co.*, **Jörg Kärcher**, Bruker AXS, introduced a program to regenerate and interactively visualize the complete reciprocal space from diffraction patterns. This program was inspired by an idea of Jim Britten; 'complete' in this context means everything pixel by pixel (or rather voxel by voxel) as recorded by the detector, not just the Bragg peaks.

With *Power Point Presentations as Warm, User-Friendly Teachers: New Tricks for an Old Dog*, **Bruce Foxman**, Brandeis, demonstrated his two sets of Power Point presentations, which allow the teaching of crystallography to undergraduates and high-school students in the absence of a teacher. These impressive sets can be downloaded from the following URLs:

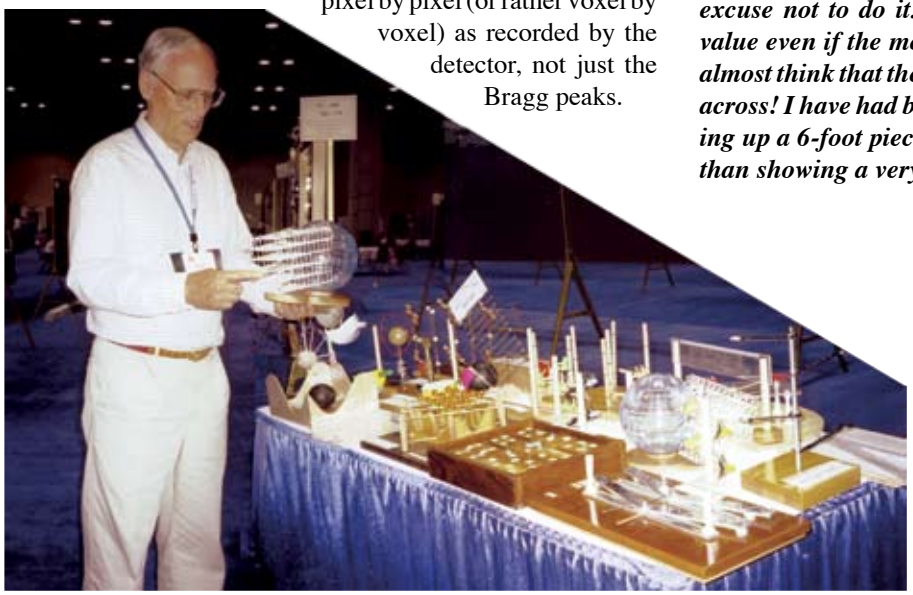
http://people.brandeis.edu/~foxman1/teaching/indexpr.html

http://people.brandeis.edu/~foxman1/teaching/indexhs.html

Finally, **Henk Schenk**, U. Amsterdam, spoke about *How to Teach the Phase Problem and the Basics of Direct Methods* and demonstrated his legendary phase problem overhead transparencies. Pointing out the obsolescence of overhead projectors (it had not been easy to organize an overhead projector for his presentation!), Henk also showed how to "translate" the phase problem transparencies into a Power Point presentation, still a work in progress.

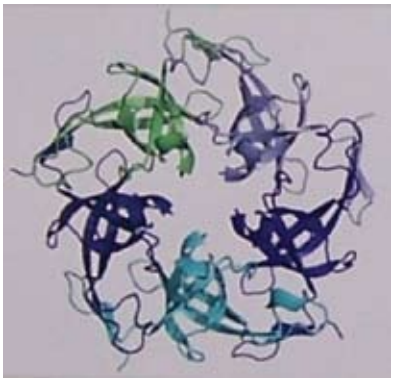
Wally Cordes who could not attend the session, sent an e-mail to the organizer: ***Anyone who gets to teach a structure-determination class should feel a need to make at least one model for each class period. The material is such that it is not at all hard to think of what might be modeled, so that there is little excuse not to do it. There is educational value even if the model is really grubby. I almost think that the cruder the model the better it gets the point across! I have had better luck in a general chemistry class holding up a 6-foot piece of venetian blind cord to talk about DNA than showing a very intricate video of the molecule.***

Peter Müller

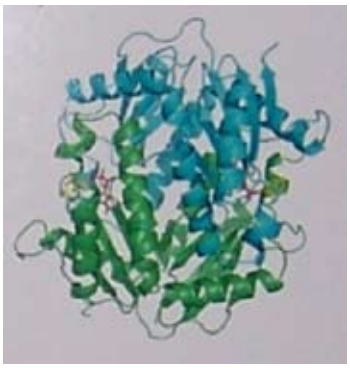


Wally Cordes showing his models at a poster session, the San Antonio ACA meeting, 2002.

Macromolecular Posters of Biological Interest



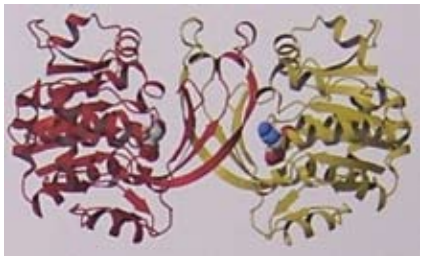
The poster session included more than a score of new macromolecular structures. Among them was a report by **Shiho Tanaka** et al., UCLA, **MP006**, on the 2.7 Å crystal structure of the CcmL subunit of the bacterial carboxysome. The carboxysome, a 1000 Å diameter microcompartment involved in carbon fixation, has a structure similar to that of a viral capsid. The CcmL subunit forms a pentameric assembly, suggesting its role as the icosahedral vertex in the microcompartment capsid. The structure, initially determined by MAD phasing, was complicated by lattice translocation disorder.



A poster by **Sue A. Roberts** et al. ,U. Arizona, **MP010**, on the 2.8 Å crystal structure of GTP Cyclohydrolase III with bound substrate, reveals a new fold and does not contain the zinc ion as seen in the other cyclohydrolases. The structure was determined by MAD phasing despite poor data due to problems freezing the crystals. Each monomer contains two similar domains with a clamshell like motif packed together to form an interdigitated dimer. There are four GTP binding sites located at the subunit interfaces.

There were several posters of medical interest. One was the report by **Anna Gardberg**, U. TN., et al., **MP007**, on the *Structures of the Immunogenic Region of Aß Complexed with Anti-protofibril Antibodies*. Aggregates of the Aß peptide are believed to be associated with Alzhheimer's disease, and antibodies to the peptide are currently in clinical trials as a possible treatment for the disease. The structure revealed that the peptide is bound to the antibody as an extended coil with multiple interactions.

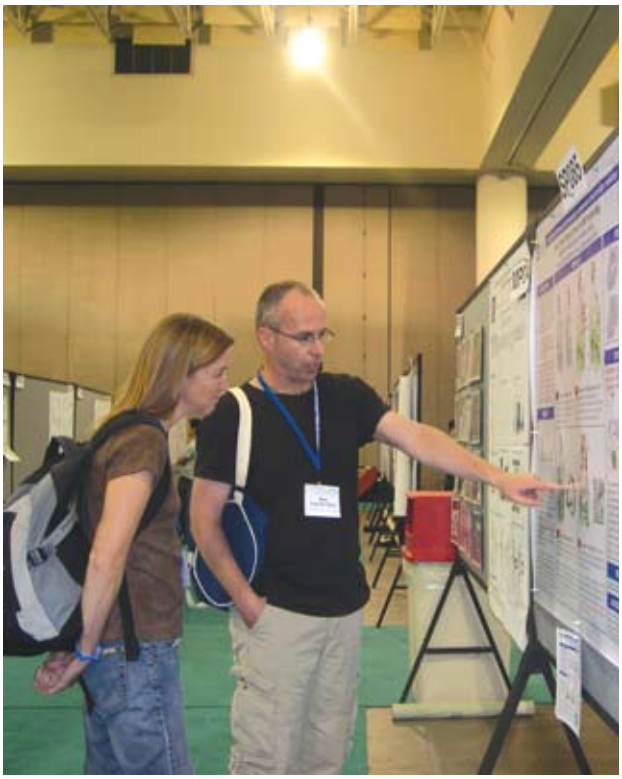
Another poster, by **Rongbao Li** et al.,Southern Research Inst., **MP033**, was on the 1.9 Å structure of the adenosine kinase from *M. tuberculosis*. This enzyme is involved in the purine salvage pathway, is structurally different from other AKs, and has a fold similar to that of ribokinase. The structures of the AK dimer with both with adenosine and an analogue were presented, showing how the active site is formed from residues from both monomers. Either inhibition of this enzyme, or the use of it to activate adenosine analogue prodrugs, may lead to an effective treatment for tuberculosis.



An interesting example of molecular ordering upon binding was provided by **Thomas Hurley** et al., Indiana U. School of Medicine, in **MP056**, which reported the structure of inhibitor-2 bound to protein phosphatase 1. The activity and functional specificity of protein phosphatases depends upon their association with regulatory and inhibitory subunits. Inhibitor-2, an intrinsically disordered protein, becomes partially ordered as it binds to the metal-binding catalytic center of protein phosphatase-1 with nanomolar affinity.

Two unusual perspectives from the RNA-protein world were also presented. **MP059** by **Charles Dann** et al., U.T. Southwestern Medical Center, described their functional and structural identification of a novel metal-sensing riboswitch from *B. subtilis*. The *mgtE* responds to magnesium binding by assuming a stable tertiary structure that assists in transcription attenuation. In **MP061**, **Matthew Miller** and colleagues, Nat. Inst. Enviro. Health, NIH, revealed the details of RNA-protein binding specificity in the Puf family of translational regulatory proteins. Members of the highly conserved Puf family bind specific RNA repeat sequences, and their results show how exceptions to the rule can fine tune the specificity of recognition.

Karl Volz and Jack Sack



Susan Buchanan and Bert van denBerg.

At the top, from left: Ross Reynolds with Madhavi Nalam; David Langley, Andrew Whitten, David Jacques, and Jill Trewhella. In the middle: Matt Miller and Xiaoqiang Wang; Tom Hurley and Allen Orville. Bottom, from left: Kevin Kirouac, Jun Wang, and Hong Lin; Ross Doyle, Peter Collins and Christine Muchmore.

Latin-American Workshop on Applications of Powder Diffraction

Campinas, São Paulo, Brazil, April 16th-20th, 2007

Specialists in the powder diffraction technique were invited to the LAWPD to give plenary lectures describing the state of the art of theory, computer methods and experimental methods.

The more than 100 participants included researchers, young scientists and students from North, Central and South America (USA, Canada, Colombia, Uruguay, Peru, Venezuela, Brazil, and Argentina) got together for a two-day Mini-Course and an Applications Workshop. Poster sessions were run during the four days of the event.

At right, soccer game: two young participants with, from left:Leopoldo Suescun, Brian Toby, Arnt Kern, Simon Billinge, Stefan Kyscia.

Lecturers & some organizers, from left: Carmelo Giacovazzo, Jim Kaduk, Simon Billinge, Brian Toby, Bob von Dreele, Peter Stephens, Bill David, Andy Fitch, Armel Le bail, Silvia Cuffini, Iris Torriani, Ernesto Estevez-Rams, Eduardo Granado.

Most of the presentations of the mini-course were recorded (voice + computer screen), and are available on the web. at: **www.lnls.br/lawpd**; click *Recorded Lectures* and choose the title from this distinguished list:

Peter Stephens

From left: Ricardo de Maura Silva, Leopoldo Suescun, Peter Stephens, Simon Billinge, Carla Azimonte, Arnt Kern, Jim Kaduk; below: Poster Session.

Peter Stephens: Powder to the people.
Andy Fitch: Experimental procedures.
Jim Kaduk: Phase identification with powder diffraction.
Peter Stephens: Tutorial on the physical and mathematical descriptions of powder diffraction lineshapes.
Carmelo Giacovazzo: Space group determination and *ab initio* phasing in EXPO2007.

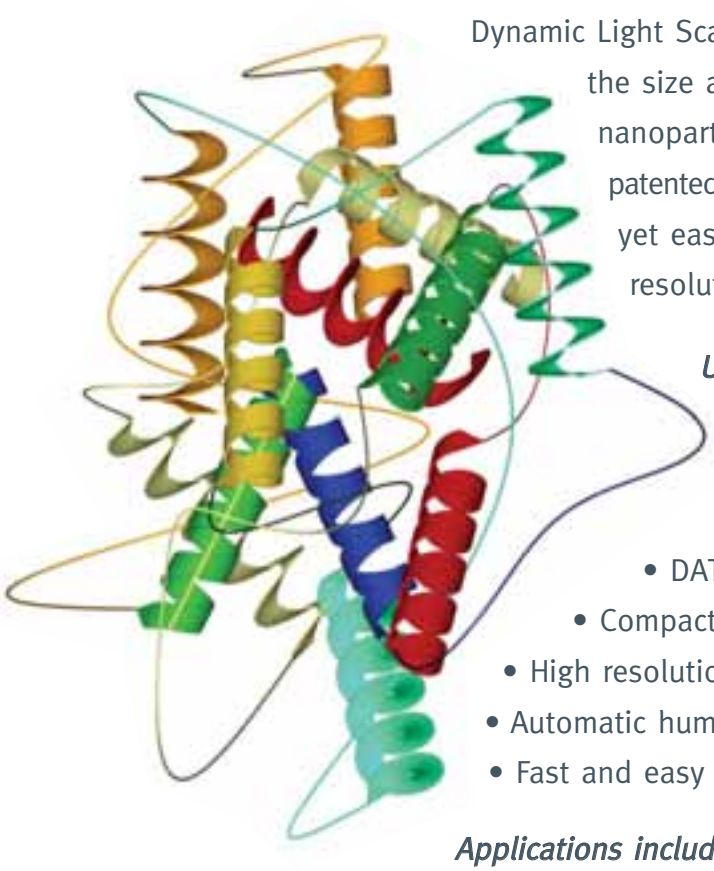
Brian Toby: A casual introduction to least-squares fitting: A [mostly] descriptive approach.
Bob Von Dreele: Refinement strategies in the Rietveld Method.
Juan Rodríguez-Carvajal: Introduction to magnetic structure determination and refinement using neutron powder diffraction.
Simon Billinge: The Atomic Pair Distribution Function method: beyond the crystal structure.
Brian Toby: Judging quality in Rietveld fits: R-factors and graphical analysis.
Carmelo Giacovazzo: EXPO2007: a powerful tool for crystal structure solution and refinement from powder data.
Bob Von Dreele: GSAS & EXPGUI and GSAS Demo: SeqGSAS & Seqplot.
Brian Litteer: Advances in transmission powder x-ray diffraction.

This event was a great success. The Organizing Committee, chaired by **Eduardo Granado**, from Unicamp / LNLS, did a wonderful job.

The organizers gratefully acknowledge the sponsorship of several institutions and commercial firms: the Laboratório Nacional de Luz Síncrotron (LNLS); the IUCr; the Brazilian Crystallographic Association (ABCr); the Research Foundations of the State of São Paulo (FAPESP); and of Minas Gerais (FAPEMIG); Centro Latino Americano de Física (CLAF); the ICDD; Bruker AXS; Rigaku Corp; and Panalytical. A soccer match organized the day of a visit to the Synchrotron Lab, between the "locals" and the "visitors" (see photo, opposite page) was a big hit. There is no agreement as to who were the winners of this match, but the crystallographic community has no doubt that they were all winners in this singular event.

Iris Torriani & Eduardo Granado

Protein Characterization by Single-Mode Fiber DLS



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Engineering of Crystalline Materials Properties, Erice, June 7-17, 2007

The 39th Course, directed by **Juan Nuova**, attracted 118 participants from 35 countries. This was a NATO Advanced Study Institute (NATO-ASI) course. The goal was to bring together crystallographers with different expertise in an environment conducive to the exchange of ideas on the design of new materials having tailor-made properties. New materials are expected to play a key role in future technologies, and a comprehensive review of technologies is a way of promoting NATO leadership in defense and security matters. Co-Directors **Lia Addadi** and **Dario Braga** emphasized this aspect in their introductory presentation.

New materials are now evident in areas that were considered not accessible previously. The rational design of materials demonstrating properties of interest will improve the prospect that they will be used in areas relevant to defense and security. For example, some new molecule-based magnets, known to possess magnetic properties well above room temperature, could be used to substitute for metal-based magnets in places where lower weight and/or malleability is at a premium, and these can be designed to have other desirable properties, such as the use of polarized light to control their magnetism. In many cases these new solids are crystalline and therefore lend themselves to careful structure analysis. Hence, the design of these materials is an aspect of what is currently known as Crystal Engineering, and the IUCr has generously contributed to the support of the school.

The scientific program was comprised of lectures on different types of materials complemented by shorter presentations (a total of 43 talks). Talks were ordered within each discipline according to an increasing level of difficulty. There were two poster sessions, each with 32 posters. A panel discussion about current problems and future trends in materials design, including defense and security issues, was organized. Each lecture allowed ten minutes for questions from students, and these were encouraged by the chair and given priority. The participation by students and the quality of their questions was very high, which resulted in the award of several prizes to young researchers during the closing ceremony (two awards to students asking the best questions during the discussion and two awards to the best poster presentation).

Adapted from a report by Juan Novoa that was slightly modified by Lodovico Riva di Sanseverino

Lodovico Riva di Sanseverino
Photo by Marco Polito.

Photo by Ulrich Baisch.

65th Annual Pittsburgh Diffraction Conference

25th, 26th, and 27th October 2007

Hauptman-Woodward Institute, Buffalo, New York

http://www.hwi.buffalo.edu

Visit http://pittdifsoc.org or contact Robert Blessing: blessing@hwi.buffalo.edu

SCIENTIFIC SESSION TOPICS

High Throughput Biomolecular Crystallization and Crystal Growth Optimization
organized by Joseph Luft, HWI, luft@hwi.buffalo.edu

Technical Advances in Biocrystallography with Synchrotron X-Rays and Spallation Neutrons
organized by Edward Snell, HWI, esnell@hwi.buffalo.edu

Biomolecular Dynamics in Crystals
organized by George Phillips, U. Wisc., phillips@biochem. wisc.edu

Small Angle Scattering Analysis of Biomolecular Structures
organized by Wayne Schultz ,HWI, schultz@hwi.buffalo.edu

Crystal Structures by Powder XRD and XRD Phasing by Charge Density Flipping
organized by Robert Von Dreele, APS, IPNS, Argonne, vondreele@anl.gov and John Spence, Ariz. State U., spence@asu.edu.

ACCOMMODATIONS

DoubleTree Club Hotel
125 High Street, Buffalo, NY
716-845-0112
http://doubletree.hilton.com

A block of rooms at $85 per night (tax included, $8 valet parking not included) is being held until 10th October for the PDC The hotel is a 5 min walk from HWI, and a 20 min, $20 taxi ride from the Buffalo-Niagara Airport. Please reserve directly with the hotel.

ACA 2008 May 31st – June 5th

Knoxville Convention Center, Knoxville, TN

Abstract Deadline: December 15, 2007

Student and Young Scientist Grant Applications: December 31, 2007

Advance Registration Deadline: April 4, 2008

Advance Hotel Registration Deadline: April 15, 2008

Register online and see Call for Papers online at

www.AmerCrystalAssn.org

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Fax: 865-574-6080

PROGRAM CHAIRS

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Dean Myles
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865-574-5662
aca08@ornl.gov
Fax 865-574-8363

Workshops, Saturday, May 31st

See meeting website link from ACA website: www.AmerCrystAssn.org

Award Symposia

Pattterson Award in honor of Bi-Cheng Wang,
organized by John Rose and Gary Newton and sponsored by the BioMac SIG

Margaret C. Etter Early Career Award to honor Radu Custelcean,
organized by Anna Gardberg and sponsored by the General Interest and Young Scientist SIGs

Transactions Symposium

on Complementary Methods,
organized by Carrie Wilmot and sponsored by the BioMac, General Interest, Neutron Scattering, Powder Diffraction, SAS, and Synchrotron SIGs

Scenic photos of the Smoky Mountains from www.nps.gov/grsm/photosmultimedia/index.htm

OCTOBER 2007

25-27 **65th Annual Pittsburgh Diffraction Conference**, Hauptman-Woodward Institute, Buffalo, New York. **www.hwi.buffalo.edu; http://pittdifsoc.org.**

NOVEMBER 2007

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

JANUARY 2008

23-24, **Advances in Protein Crystallography,** Palm Springs, CA. **www.selectbiosciences.com/conferences/APC2008/**

MAY 2008

29-June 8 **From Molecules to Medicine, Integrating Crystallography in Drug Discovery** Erice, Italy. **www.crystalerice.org/erice2008/2008.htm.**

JUNE 2008

3-6 **16st Annual Meeting of the German Cristallographic Assoc.**, Erlangen, Germany; **http://conventus.de/dgk2008/**; Contact: Herr Prof. Dr. Andreas Magerl, Friedrich-Alexander Universität Erlangen-Nürnberg, +49 (0) 9131 85 25 181; **andreas.magerl@krist.uni-erlangen.de.**

31-June 5 **ACA Annual Meeting - Knoxville, TN** ***Local Chair: Jason Hodges, ORNL, Program Chairs: Paul Butler, NIST, and Dean Myles, ORNL,*** **aca08@ornl.gov.**

AUGUST 2008

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

JUNE 2009

4-14 **High Pressure Crystallography: From Novel Experimental Approaches to Applications to Cutting Edge:** Erice, Italy. **www.crystalerice.org/2009.htm.**

JULY 2009

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

AUGUST 2009

9-14 ECM-25 Istanbul, Turkey.

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