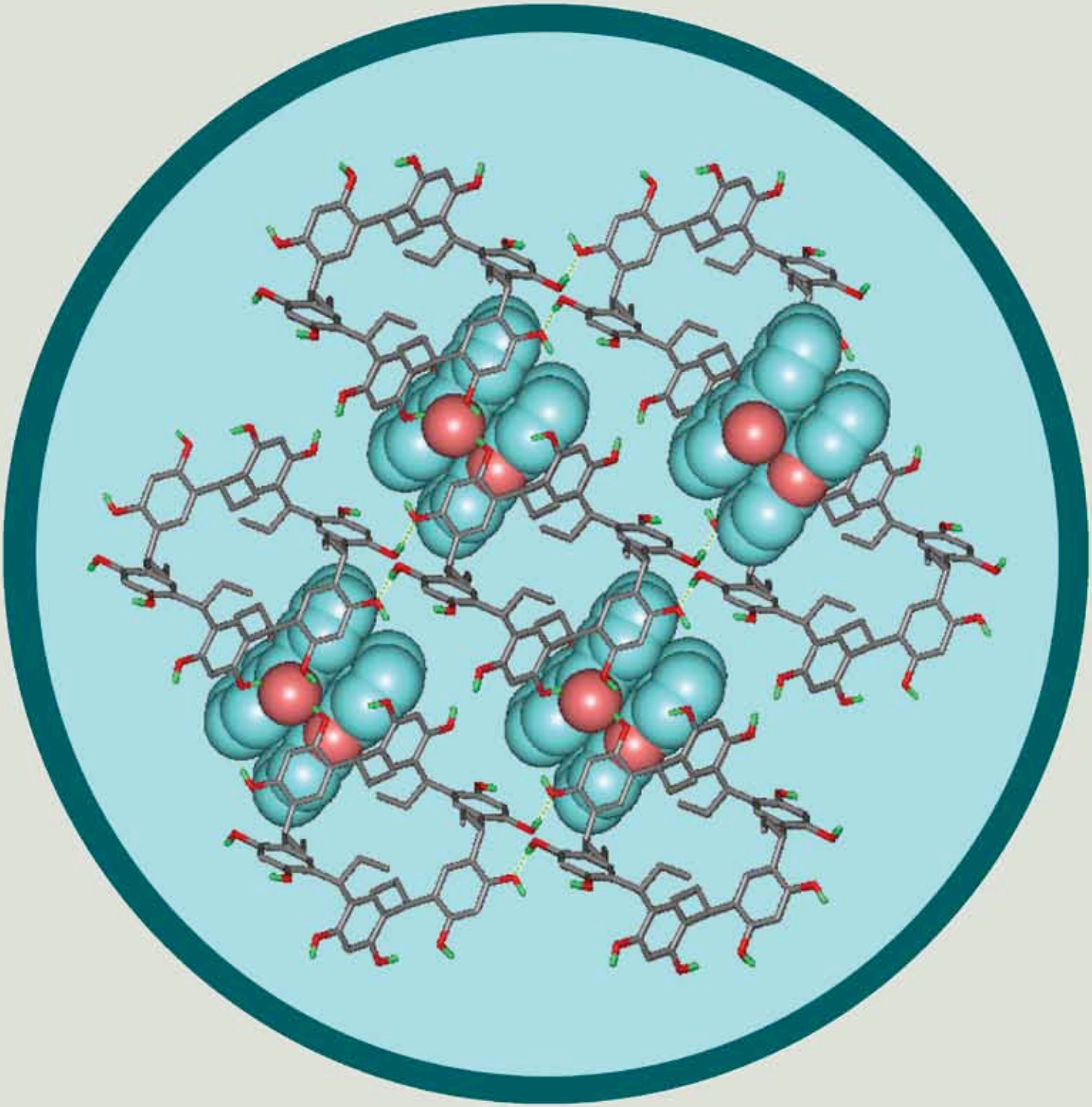
ACA RefleXions

American Crystallographic Association

Number 3
Fall, 2009



The 2009 ACA Meeting in Toronto

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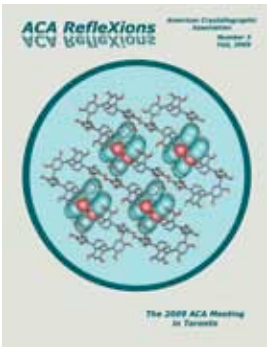
Cover: see page 10.
Image from the plenary lecture by Philip Coppens at the 2009 ACA meeting in Toronto



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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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Wow, what a wonderful ACA Annual Meeting in Toronto! Many thanks to Jim Britten as Program Chair and David Rose as Local Chair for putting together such a splendid meeting. There were over 900 people registered, making it one of the larger ACA meetings. Look elsewhere in this issue of *RefleXions* for details and pictures. There were several innovations at this meeting. We distributed a CD containing all the abstracts and a small program book instead of the larger (and far more expensive) abstract book. We gave attendees very useful hard cover folios complete with note pads (thanks to Bruker-AXS) and pens (thanks to Hampton Research); attendees had been advised (via a tip on the website) to bring their own bags from a previous meeting. We began each day with an unopposed plenary session which was followed by simultaneous sessions organized by the SIGs. This seemed to work very well - we will use the same plan next year in Chicago.

Two workshops were held; one dealt with twinned macromolecular crystals, and we thank Bristol-Myers-Squibb, Hewlett-Packard and Bruker-AXS for making it possible to use laptops --see the note below. The other, on incommensurate structure analysis using the JANA2006 software, was a two-day workshop, a first at ACA meetings.

For at least nine years the next ACA meeting program has been put together on the Friday following the meeting. Ross Angel (Program Chair for Chicago) and about 20 SIG representatives met with some members of Council and laid out the entire session schedule for Chicago. It already looks to be just as good as the one we just held.

In a few weeks you will be receiving in the mail a package with ballots plus your annual dues notice. Please don't throw it out! You are asked to choose between two excellent candidates for ACA Vice-President (Tom Koetzle and Jim Britten) as well as selecting one candidate for each of the ACA Standing Committees; Bernie Santarsiero is unopposed for a second term as treasurer. Please read their statements and vote! Voting can easily be done on line at the ACA web site (***www.AmerCrystalAssn.org***); you will need your member number to do this - it is in your election materials and on your dues statement. The ballots also list the candidates for SIG officers. I encourage each of you to join one or more SIG; there is a check list in the dues form for the SIGs you wish to join. I strongly urge you to go to those SIG meetings in Chicago and help plan for the ACA meeting in New Orleans in 2011. The SIG meetings are typically held just after the sessions end, either in the morning or afternoon; your SIG representatives will then go to the Friday meeting armed with your ideas for sessions in New Orleans.

In the election package there will be a ballot for you to decide for or against an ACA Fellows program modeled after similar ones in other societies (ACS and MSA, for example). This is a program to honor those of you who have provided exemplary service to crystallography- it would be an award, not a membership category. In the first couple of years more Fellows would be elected to build up numbers and then this would be reduced in later years. Their ranks would be filled via nominations from you, the membership; details will be in the ballot. Please vote!

In the package you will see some small adjustments in ACA dues. Regular member dues remain at $100 per year; dues for postdocs and retired members are now identical - $40; and student dues are $25. Moreover, the postdoc category is now permitted for 10 years past the PhD; formerly the limit was 5 years. I encourage everyone to pay dues; this can easily be done on line at the ACA web site. Again you will need that member number. Note that the dues form gives you the opportunity to make contributions to the various ACA award funds; any amount is most welcome. You should know that the funds are carefully overseen by Bernie Santarsiero and S.N. Rao, our Financial Officer. We actually made ~5% on our investments during this recession!

Finally, note that the Council decided, considering the best interests of all, that the ACA will hold a spring meeting in 2014 as is normally done in the year when an IUCr Congress occurs, despite the relative proximity of Montreal. The location is yet to be determined but is likely to be in the far west.

Bob Von Dreele

Laptop computers available for ACA-related activities

The laptop computers used in the twinning workshop in Toronto came from two sources: Bristol-Myers Squibb donated 30 IBM T42 ThinkPad laptops to the ACA for use in this, and subsequent workshops/activities (these laptops are now with Bernie Santarsiero in Chicago and are available for any use deemed suitable by the ACA Council (e.g. workshops at the Chicago ACA meeting next year; Bill Duax and his summer high-school students). In addition Hewlett-Packard loaned four high-end laptops (one for each instructor and one spare).

Bruker-AXS kindly agreed to bring the laptops to Toronto from Madison, WI and back with the Bruker gear. This assistance saved the workshop about $900 (our quote to ship the computers to Toronto through Marcia in Buffalo was $1,200 minus the cost of $300 to ship the computers domestically to Madison to be paid out of the workshop budget). In fact, without this assistance, it would not have been possible to bring the laptops to Toronto on the workshop budget. Because of the uncertainty of whether or not BMS would be able to transport the laptops, they were not advertised as available in advance, and they were therefore underutilized. Even with less analysis of participant data than hoped, the feedback received so far suggests that the twinning workshop was successful.

The twinning workshop was the first (and only) ACA function to use these laptops so far. However, organizers / instructors are encouraged to direct requests for access to the ACA Council. They are loaded with Linux and some crystallographic software (e.g. CCP4, PHENIX, SHELX).

Herb Klei

ACA Office Costs I: How to Communicate Better in the 21st Century

In the summer *RefleXions*, I discussed the telecommunications part of the ACA meeting budget. Now I'll discuss office costs relating to several aspects of communication, including the costs in printing and mailing out *RefleXions*, building and supporting the ACA website, and outreach to the membership. One of the major costs that continues to rise is postage. *RefleXions*, information on the upcoming national meeting, membership renewal notices, and ballots are all distributed by (snail) mail. Is this the most practical and useful form for communication?

The finance committee met with the ACA Council in Toronto to consider how we can communicate better in the 21st Century. With *RefleXions*, Judy and Connie do a wonderful job of assembling an attractive publication. Is this something that members find interesting and useful in its present form? In general the response has been extremely favorable about keeping the printed form, and we continue to look for ways to reduce costs while producing an outstanding, high-quality printed publication. Printing costs have maintained relatively flat (due in large part to the way the editors assemble the issues) while postage costs have tripled over the past decade. Ad income continues to drop from a high point five years ago. Would members prefer a publication that is distributed by email? Or one only available from the ACA website in electronic form as a pdf or digital file? (See, for example, **www.zinio.com**.) How often do you currently gather information from RSS feeds, podcasts, or blogs? Should the ACA form a group on Facebook?

Would the majority of the membership prefer the option of a website that allows individuals to routinely vote, register, and respond more easily online? Would some form of a blog enable the membership to carry out extended discussion on various topics relating to ACA business and scientific discovery? Vendors are also major contributors to the ACA and the national meeting. Is *RefleXions* and the ACA website useful to you? Should we include a section that will promote and highlight vendors? How can we encourage vendors to sponsor more awards, sessions, and events at the national meeting? How can we attract even more vendors and sponsors to our national meeting?

These are all options that we are willing to explore, though it might take some time to ramp up our resources to move in a certain direction. Most of these options would be cost-effective, but we want to hear from you.

We are in the early stages of generating a new ACA website. The goal is to make the information more accessible, complete, and useful. Are you getting all of the information you need from the ACA website? What's missing? We wish to include more on the history of the ACA, audio archives of award lectures, and a broader multimedia foundation to make the *Transactions*, plenary lectures, and other resources accessible, and to have a broader impact on education, research, teaching, and science funding and policy issues. We hope that this expanded website will benefit the membership and the crystallographic and scientific communities. In terms of outreach, we are working with the AIP to promote greater visibility of the ACA beyond the membership.

As always, please email me, or any member of the ACA Council, with your comments, concerns, and ideas.

Bernie Santarsiero, ACA Treasurer, ***bds@uic.edu***

ACA Fellows

The ACA Council has discussed at length the designation of certain ACA members as ACA Fellows. Each of our ACA Awards is defined by very narrow criteria; this member designation would allow us to significantly recognize and honor excellence in a broader cross-section of the membership than is currently possible. Some of the details were presented at the ACA Business meeting in Salt Lake City, and outlined in *RefleXions* (Fall 2007, page 9). The ACA Council revisited the proposal this year, and decided to move forward with a vote by the membership. Many scientific organizations and societies have similar member designations: Mineralogical Society of America, Microscopy Society of America, American Association for the Advancement of Science, Chemical Institute of Canada, American Institute of Chemical Engineers, and the American Physical Society. As recently as last year, the American Chemical Society established a similar designation to recognize members "for outstanding achievements in and contributions to Science, the Profession, and the Society." Unlike our ACA Awards, the nomination of an individual as an ACA Fellow not only recognizes their high level of excellence in scientific research, teaching, and professional duties but also their service with distinction in the ACA. We view ACA Fellows as ambassadors for crystallography, science, mathematics, and engineering to the general public and scientific community, AND wish to recognize their outstanding leadership and engagement in the ACA. We hope that eventually about 10% of the membership would be recognized as ACA Fellows; we will announce our new inductees and honor all ACA Fellows during the Awards Banquet at our national meetings. We urge you to vote in the coming election.

Judy Flippen-Anderson and Bernie Santarsieto

Editor's note: Because Judy and Bernie did not mention which organizations under the AIP umbrella did NOT have a Fellows membership designation, I did some web research. The American Geophysical Union also has a Fellows category, as does the Optical Society of America; the American Astronomical Society does not, and the Society of Rheology does not. Broading my search, I found that the Protein Society does not either. The American Mathematical Society has a very interesting FAQ web page on the subject: www.ams.org/secretary/fellows-info, in which they report that their 2006 ballot failed by a small margin; since then the governing body has revisited the subject and they were to propose it again in 2008, taking into account the issues raised by members and also benefiting from the experience of other societies.

Connie Rajnak

A Bright Future for Neutron Crystallography

It is an exciting time for neutron crystallography with powerful new facilities coming on line and providing unparalleled capabilities. This is a good opportunity for a *RefleXions* column with a brief description of some of the noteworthy new instruments. In the limited space that is available it is only possible to hit a few of the highlights here, focusing on U.S. and Canadian neutron scattering facilities. Readers who are interested in additional information, and in facilities outside North America, may wish to consult the facilities' own websites. A good starting point is accessible from the home page of SNUG (the Synchrotron and Neutron Users' Group, **www.snugroups.org**).

The SNS (Spallation Neutron Source) at Oak Ridge, now in its third year of operation, is currently the world's highest-power pulsed neutron source. Last year, during the Knoxville ACA meeting, many ACA members had an opportunity to see the SNS first-hand. A rapidly expanding user community is developing at Oak Ridge around the SNS and the newly upgraded experimental facilities at the HFIR (High Flux Isotope Reactor). At the SNS, the instrument suite will include several single-crystal diffractometers - TOPAZ, optimized for chemical crystallography, and MaNDi, designed for macromolecular structures, as well as the SNAP diffractometer for high-pressure work. A third-generation powder diffractometer, POWGEN3, is also under development. The SNAP instrument is currently accepting users; the scientific programs at POWGEN3 and TOPAZ are expected to commence next year, while ManDi is expected to be available in 2014. All four instruments will offer unique capabilities. For example, on the TOPAZ instrument it will be possible to carry out high-resolution neutron structure determinations using nearly "x-ray size" crystals with data obtained in a matter of hours, and in the future, a neutron spin polarization option will be provided for studying magnetic systems. The SNAP instrument features state-of-the-art opposed anvil high-pressure cells and allows studies of a variety of powder and single-crystal samples under extreme conditions of pressure and temperature. MaNDi will be a state-of-the-art high-resolution diffractometer, optimized for rapid data collection from crystals of large structures. The MaNDi instrument will complement the capabilities of the highly oversubscribed PCS at the Lujan Center, Los Alamos, which presently is the only macromolecular neutron diffractometer operating in North America. In addition a new quasi-Laue diffractometer, IMAGINE, is under development for the HFIR. The availability of the SNS and HFIR instrument suites alongside the facilities at the Lujan Center, as well as those at the NCNR (National Center for Neutron Research) at NIST and the NRC-Canadian Neutron Beam Centre at Chalk River*, suites which include beamlines for powder diffraction, small-angle scattering, reflectometry, and residual stress analysis, will support a dramatic expansion in the use of neutrons in North America for a wide range of applications. The future of neutron crystallography is bright indeed, and a host of exciting new possibilities beckon.

Tom Koetzle

**** The NRU reactor at Chalk River is currently shut down while undergoing repairs that are expected to be completed by the end of the first quarter of 2010. Proposals for beam time at the Canadian Neutron Beam Centre are still encouraged because it is the intention to be running approved user projects, especially those for Canadian academic users, immediately upon restart of the reactor.***

Editor's note: Tom is a Senior Chemist at the Brookhaven National Laboratory (retired); a former special term appointee at the Argonne National Laboratory, and Scientific Secretary of the instrument development team for TOPAZ at ORNL's SNS. He has promised to correspond by email with researchers at the various neutron and synchrotron facilities and to edit a section in the spring 2010 RefleXions.

2010 Art in Crystallography Contest

We are accepting entries to the **2010Art in Crystallography Contest** in the form of images emailed to either Editor (**conniechidester@earthlink.net** or **flippen@rcsb.rutgers.edu**). Entries should be accompanied by a paragraph explaining the science and the method of producing the image. A photo of the artist would be appreciated but is not required. Prizes consist of small monetary awards and banquet tickets at the annual meeting. Winning entries will be posted on the web and will be displayed at the ACA Meeting. (Winners are not required to attend the meeting). We will also feature images in *ACA RefleXions* from time to time; the 2009 entries were featured on the cover of the *IUCr News* in the issue 17, #2. Please let us know if you are interested in being a judge. **The deadline for 2010 Contest is May 1st, 2010**

Reminder !

Look for 2010 dues invoices and ballots to arrive in your mailbox soon

Appeal for Volunteers

***RefleXions* Editors Judy and Connie are continuing an appeal to ACA members to volunteer for the *RefleXions* staff. This issue we are proud to announce that Bomina Yu is our new News and Awards section chief. (See the following announcement.) Also, Tom Koetzle, who has the Guest Editor spot in this issue, has agreed to correspond by email with researchers at the various Neutron and Synchrotron facilities and to edit a section in the spring *RefleXions*, much as Carrie Wilmot did (on Etter Award winners) in the spring '09 issue. Judy and Connie are volunteers, and so is our staff photographer, Peter Müller. We can envision volunteers in charge of the *Books* section; the *Opinion* columns; the *Calendar; Meeting Reports; Future Meetings;* or Wilmot /Koetzle type articles on topics including but not limited to: crystallography education, nanoscience, PDF theory & techniques, or SAS. Note that we don't do all of these sections in every issue. The *Books* section appears in two issues; *Opinion* columns are about twice a year and have up to now included global warming updates and threats to the scientific teaching of evolution. *Meeting Reports* and *Future Meetings* are in every issue, but the editor's work is limited to editing for style and content since reports, meeting flyers and photographs are contributed by meeting attendees. If you have an inclination to make our dream a reality, please contact either of us: Judy Flippen-Anderson <flippen@rcsb.rutgers.edu>, or Connie Rajnak, <conniechidester@earthlink.net>.**

2010 ACA Trueblood Award to Ton Spek

This award was established by the ACA in 2001 in memory of **Kenneth N. Trueblood.** Professor Trueblood taught at UCLA from 1949 to 1998, where he was recognized as an outstanding teacher and mentor. His early use of computers and development of crystallographic computer programs facilitated the examination of chemical and molecular details of many structures at the frontiers of research. In a similar fashion, the **ACA Trueblood Award** recognizes exceptional achievement in computational or chemical crystallography.

Anthony L. Spek has been selected to receive the 2010 award for his *Outstanding contributions to chemical crystallography and crystallographic computing, in particular the ongoing development of the program PLATON to facilitate the control, analysis, validation and graphical representation of small molecule crystal structures*. Anthony Spek is a Professor in Chemical and Computational Crystallography at Utrecht University Bijvoet Center for Biomolecular Research in the Netherlands. Members of the selection committee were: **Angus Wilkinson, Lachlan Cranswick and Alan Pinkerton.**

Bomina Yu Joins ACA RefleXions Staff

Judy and Connie are pleased to announce that **Bomina Yu**, Columbia University, has joined our volunteer staff as Awards & News editor. She did the entire Awards & News section in this issue. Please add Bomina Yu **by2112@columbia.edu** to all appropriate distribution lists.

Etter Early Career Award to Ray Trievel

The **Margaret C. Etter Early Career Award** was established in her memory to recognize outstanding achievement and future potential in crystallographic research demonstrated by a scientist at an early stage of their independent career. **Raymond C. Trievel** will receive the 2010 award at the ACA annual meeting in Chicago. Ray Trievel is an Associate Professor of Biological Chemistry at the University of Michigan where he is investigating the molecular mechanisms underlying protein modifications and their regulatory roles in gene expression and signal transduction. His achievements in elucidating the substrate specificity and catalytic mechanism of histone methyltransferases in the short time that he has been an independent researcher have earned him the **2010 Etter Early Career Award.**

David Eisenberg Receives Harvey Prize

At a ceremony held March 23, 2009 at the Technion-Israel Institute of Technology, **David Eisenberg** received the **Harvey Prize** in Human Health for his seminal work on the structures of amyloids and prions. As well as being a Howard Hughes Medical Institute (HHMI) investigator and renowned crystallographer, David Eisenberg is a Professor of Chemistry, Biochemistry and Biological Chemistry at UCLA and Director of the UCLA-DOE Institute for Genomics and Proteomics. The Eisenberg lab focuses on structurally characterizing the pathologies of amyloids and prions, and the structural biology of *Mycobacterium tuberculosis*, with particular focus on protein-protein complexes. His contribution to the understanding of the fundamental properties of the fibrous proteins associated with neurodegenerative diseases, including Alzhemer's, Parkinson's, and Creutzfeldt-Jakob diseases, earned him this year's Harvey Prize.

First awarded in 1972, the annual Harvey Prize celebrates outstanding efforts in science, technology, health and peace. Named after and established by the late Leo M. Harvey, an American Technion Society supporter from Los Angeles, the prestigious Harvey Prize is considered a good predictor of the Nobel Prize, with eleven of its recipients going on to win the Nobel.

John Kuriyan Receives ASBMB Merck Award

The American Society for Biochemistry and Molecular Biology (ASBMB) honored **John Kuriyan** with the **2009 Merck Award**, which recognizes outstanding contributions to research in biochemistry and molecular biology. Kuriyan is a HHMI investigator and Chancellor's Professor at UC Berkeley. One of the world's leading researchers on the structure and function of protein kinases, his studies of c-Src, c-Abl, and CaMKII have provided exciting new insights into the structure and function of molecular systems that are similar to those found in many other biological contexts. Kuriyan's laboratory has also made pioneering discoveries in the field of processive DNA replication. His award lecture, ***Allosteric Mechanisms in Receptor Tyrosine Kinase Activation***, was presented at the ASBMB annual meeting in April. ***From ASBMB Today June 2009***

John Kuriyan (right) accepts the ASBMB-Merck Award from Gregory Petsko.

David Davies is awarded the Tabor JBC Lectureship

The **Herbert Tabor/Journal of Biological Chemistry Lectureship** has been established by the **American Society for Biochemistry and Molecular Biology** to recognize the many contributions of editor Herbert Tabor to the *Journal of Biological Chemistry* and the society. This year's recipient was **David Davies** of the National Institute of Diabetes and Digestive and Kidney Diseases at NIH in honor of his outstanding achievements in crystallography. Davies presented his lecture, ***Fifty years of Protein Structure: From Myoglobin to the Innate Immune System,*** at the ASBMB annual meeting in April.

John Grinnell, Cadmus Communications (left) presents the Herbert Tabor/JBC Award to David Davies.

Linus Pauling Medal to be Awarded to Stephen Lippard

Stephen J. Lippard, Arthur Amos Noyes Professor of Chemistry at MIT, will receive the **2009 Linus Pauling Medal** from the Puget Sound, Oregon, and Portland Sections of the ACS this November. The annual award recognizes outstanding accomplishments in chemistry in the spirit of Linus Pauling, a native of the Pacific Northwest. Lippard is being honored for outstanding contributions to chemistry meriting national and international recognition. Structural and mechanistic studies of macromolecules as well as synthetic inorganic chemistry in the Lippard laboratory focus on the synthesis, reactions, physical and structural properties of metal complexes in their natural systems and as models for the active sites of metalloproteins and as anti-cancer drugs.

Francis Collins Appointed NIH Director

On August 17, 2009, **Francis S. Collins**, M.D., Ph.D. became the 16th director of the National Institutes of Health. Collins, a physician-geneticist noted for his landmark discoveries of disease genes and his leadership of the Human Genome Project, served as director of NIH's National Human Genome Research Institute (NHGRI) from 1993-2008. Under his direction, the Human Genome Project consistently met projected milestones ahead of schedule and under budget. This remarkable international project culminated in April 2003 with the completion of a finished sequence of the human DNA instruction book.

Collins received a B.S. in chemistry (U. Virginia), a Ph.D. in physical chemistry (Yale), and an M.D. with honors (U. North Carolina). Prior to coming to the NIH in 1993, he spent nine years on the faculty of U. Michigan, where he was a Howard Hughes Medical Institute investigator. He is an elected member of the Institute of Medicine and the National Academy of Sciences. In 2007 he was awarded the Presidential Medal of Freedom.

Clifford G. Shull – Fellowship Program

The Neutron Scattering Science Division at Oak Ridge National Laboratory (ORNL) announces the establishment of the **Clifford G. Shull Fellowship**. Co-recipient of the 1994 Nobel Prize in physics, Shull began his work in 1946 at what is now ORNL. He has been called the "Father of Neutron Scattering," and this fellowship has been established in recognition of his pioneering work in this field.

The goal of the fellowship is to attract new scientific talent to ORNL for the development of its neutron science program; candidates with exceptional ability who are capable of developing innovative research programs and who show the promise of outstanding leadership. Shull fellows will be sponsored by the Neutron Scattering Science Division, which includes the Spallation Neutron Source and High Flux Isotope Reactor facilities in Oak Ridge, TN. Fellowships will be two-year appointments renewable for a third. Qualifications: PhD minimum; no more than 3 years past completion of PhD; not currently occupying an ORNL postdoctural position. For more information and to apply online see: ***neutrons.ornl.gov/shullfellowship***. **Applications must be received by December 13, 2009**. ORNL is an equal opportunity employer and is committed to workforce diversity; women and minorities are strongly encouraged to apply. Applicants need not be US citizens.

Case Western Reserve University receives $4M from the National Institute for Biomedical Imaging and Bioengineering to fund the CSB

The **Center for Synchrotron Biosciences**, located at Brookhaven National Laboratory in New York, operates four synchrotron beamlines that provide state of the art equipment, techniques, and user support and training for radiolytic footprinting, x-ray spectroscopy, and macromolecular crystallography experiments. The center, to be funded through 2014, has developed a number of novel structural biology tools and resources for the international scientific community to support the study of the structure and dynamics of proteins and nucleic acids. The new grant will be used to improve and continue three technology cores: a footprinting core, including novel structural mass spectrometry and proteomic tools, an x-ray spectroscopy core, and the macromolecular crystallography core. More than 175 projects across all three cores, with funding from over 200 peer-reviewed grants, will be supported by the center.

Funding Opportunity Announcements by the NIH

The **NIH Director's Pioneer Award Program** complements NIH's traditional, investigator-initiated grant programs by supporting individual scientists of exceptional creativity who propose pioneering and possibly transforming approaches to addressing major biomedical or behavioral challenges. Awardees must commit the major portion (at least 51%) of their research effort to activities supported by the Pioneer Award. See **http://grants.nih.gov/grants/guide/rfa-files/RFA-RM-09-010.html** for more information. **Applications are due on October 20, 2009.**

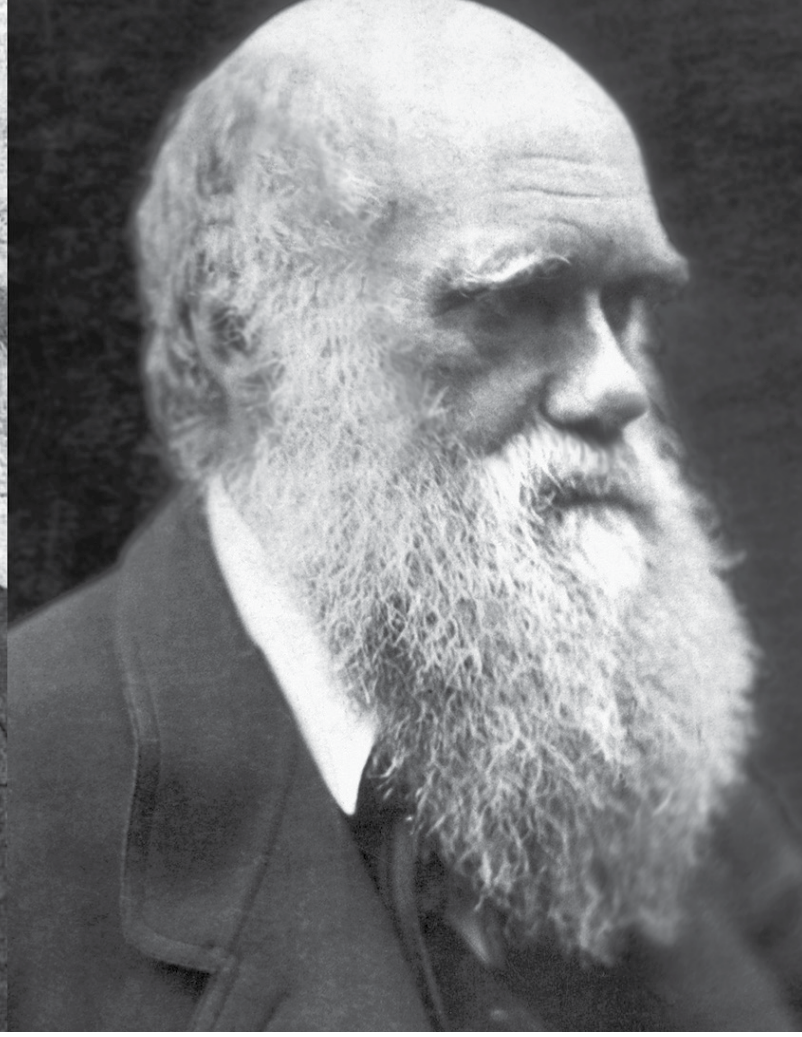
Research to Understand and Inform Interventions that Promote the Research Careers of Students in Biomedical and Behavioral Sciences, sponsored by NIGMS (National Institute of General Medical Sciences). The proposed research need not be restricted to underrepresented minority students. See **http://grants.nih.gov/grants/guide/rfa-files/RFA-GM-10-008.html** for more information. **Applications are due on October 22, 2009**.

Win a SMART X2S

Imagine being able to teach your students "hands on" crystallography. Now you can! See **bruker-axs.de/x2s-loan.html** for full contest rules and entry form. Entries will be accepted through midnight on **December 31, 2009**.

Deadline Imminent for Ludo Frevel Scholarships

To encourage promising graduate students to pursue crystallography-related research, the ICDD has established the **Ludo Frevel Crystallography Scholarship Fund.** Recipients each receive an award of $2,500. Applications for the year 2010 awards must be received by ICDD no later than 30 October 2009.See **www.icdd.com/resources/awards/frevel.htm** for qualifications and forms.



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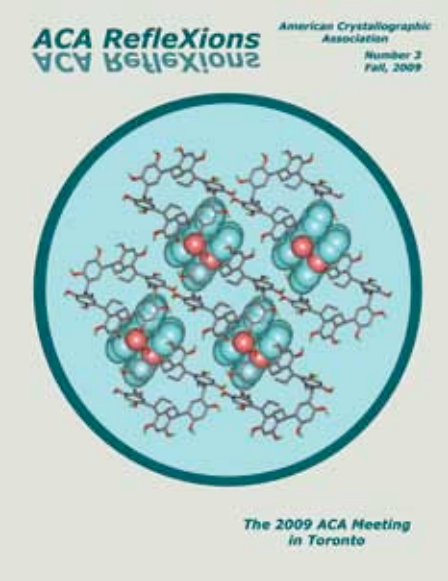


The 3-dimensional supramolecular architecture of HECR · 2 xanthone · 6 MeOH, containing dimeric xanthone, viewed along the c axis. Methanol molecules were omitted for clarity. (HECR = hexaethylresorcin[6] arene). From "Supramolecular solids and time-resolved diffraction," Philip Coppens, Shao-Liang Zheng, Milan Gembicky, Marc Messerschmidt and Paulina M. Dominiak, Cryst. Eng. Comm., 2006, 8, 735-741. © 2006, Royal Society of Chemistry.

An Image from Philip Coppens' Plenary Lecture: New Developments in X-ray Photocrystallography

For the first time, the 2009 ACA Meeting in Toronto featured plenary lectures, unopposed, every day. Philip, a Distinguished Professor of Chemistry at SUNY, Buffalo, is a former ACA President and a past president of the IUCr. Among his many awards, he received the 1994 ACA Buerger Award, the 1996 Gregori Aminoff Prize of the Royal Swedish Academy of Sciences, and the 2006 Ewald Prize of the IUCr. Sine Larson, the current IUCr President, introduced Philip.

In his lecture, Philip discussed the supramolecular solid state as a medium *par excellence* for photochemical studies of molecules in a well defined environment. The xanthone molecules are considerably diluted in the host; the molarity of the xanthone dimer is 1.752 compared to 7.106 in neat crystals. The pump-probe pulsing experiments show that in the microseconds-lifetime excited state (ES) the spacing of the molecules in the dimer decreases by 0.26 Å, to 3.15 Å, corresponding to a stronger interaction typical for excimer formation, but never before directly observed by diffraction methods. A lateral shift of 0.31Å occurs. The re-birth of Laue in time-resolved studies was also mentioned. A monochromatic stroboscopic (5000-15000 cycles/sec) image of a 1000ns total exposure was compared to single-pulse, 70ps Laue diffraction images taken at the BIOCARS beamline 14-ID at the at APS.

The cover image was also used in "Static and time-resolved photocrystallographic studies in supramolecular solids," Philip Coppens, Shao-Liang Zheng and Milan Gembicky, Z. Kristallogr., 2008, 223, 265-271. Other relevant publications are: "The New Photocrystallography," Philip Coppens, Angew. Chem., 2009, 48, 4280-4281, and "Single-Crystal-to-Single-Crystal E to Z Isomerization of Tiglic Acid in a Supramolecular Framework," Shao-Liang Zheng, Marc Messerschmidt and Philip Coppens, Acta Crystallogr. B63, 2007, 644-649.

Right: Alana Goldberg, Jason Porta, Clare Yannette, Janeth Presores.

Above, l to r: Ahmad Kanaan, Filipp Frank, and Yazan Abbas, all from McGill U. Photo by Eric Lawrence. Below: Zbigniew Dauter and Bob Sweet (right). Photo by Peter Müller.

Below: Queens U. Trio; l to r: Mark Currie, Kateryna Podzelinska, and Kristin Low. Both photos compliments of Eric Lawrence.

ACA President Bob Von Dreele, and Past President Marvin Hackert

2009 ACA Meeting in Toronto, July 25-30

Program Chair David Rose and Local Chair Jim Britten

Despite unforeseen obstacles, including a major Toronto city workers strike (including garbage collection), a short rail strike and an unusually rainy period featuring some spectacular thunderstorms, the meeting was, by all accounts, very successful. By the time the meeting ended, the strikes were settled and the weather had calmed down, a message that should be sent to all potential ACA host cities.

Jim Britten and his team organized a stimulating and appropriately broad scientific program and, as usual, the meeting organization from the Buffalo ACA staff was flawless. The pre-meeting JANA and Twinning workshops were very well received. Even in the face of the economic difficulties, ACA2009 had the third largest attendance ever, with well over 900 registrants. The major award winners, **Shih-Lin Chang** (Warren Award), **Svilen Bobev** (Etter Award) and **Michael James** (Buerger Award), along with special plenary speakers **Ted Baker** and **Philip Coppens**, all gave popular lectures, despite the early start hour. As usual, the enthusiastic and generous exhibitors showed off their latest products, made many personal connections, and sponsored some lively social occasions.

Special thanks to the excellent cohort of Canadian crystallographers who attended the meeting (many of whom helped with volunteer jobs). I think we showed the ACA that Toronto, and Canada in general,is worth keeping on the list of sites for future ACA meetings. See you in Chicago next year!

David Rose, Local Chair

Shih-Lin Chang, far left, received the 2009 **Bertram E. Warren** award in session **SP01**, for which there is no session report because his lecture *Coherent Dynamical Interaction in X-ray Multiple Diffraction and Crystal Cavity Resonance*. will be published in the spring 2010 *RefleXions*. Shih-Lin is a professor at the National Tsing Hua University in Taiwan.

SP02, page opposite, featured the 2009 **Margaret C. Etter Award** recipient, **Svilen Bobev**, center left.

Michael James, above, received the **Martin J. Buerger Award** in **SP05**, opposite page..

Other plenary lectures were given by, at far left, **Ted Baker** (see **SP03**, opposite) and, at right, **Philip Coppens,** who gave the **SP04** lecture on *New Developments in X-ray Photocrystallography: From Hours to Microseconds and Beyond*. (See the Cover, and the *On the Cover* article, page 10.)

All photographs on this page were taken by ACA staff photographer, Peter Müller. Unless otherwise noted, the speaker photos on the following pages were taken by the AV staff: l to r: Anna Rose, Matt Tammam, William Lotosky, Miguel Neves, Sherry Boodram

l to r: Greg Hogan, Gina Thede, Julie Aaron, Jason Porta, Ankit Gupta, Ivan Campeotto, Catherine Aldous, Brandon Mercado, Robert Huether. Photo by Peter Müller..

SP.02 Etter Early Career Award Symposium

The award symposium began with the presentation of **Etter Early Career Award** to **Svilen Bobev**, U. Delaware, by ACA president Bob Von Dreele. Svilen presented his work on novel germanide structures, and discussed variations in these structures with a number of atoms from the lanthanide series.

Ankit Gupta, U. Rochester Med. School, described an unknown splicing factor domain that plays a cooperative role in recognition of the 3' slice site in pre-mRNA splicing complex. **Catherine Aldous**, U. Ottawa, presented work on the whole phase diagram of the methane-nitrogen system. She observed new structures at different temperatures and pressures. **Ivan Campeotto**, U. Leeds, was the Young Scientist SIG's choice for the **Margaret C. Etter Student Lecturer** award. He discussed the use of directed evolution to locate a mutation that increased substrate specificity and stereo selectivity of N-acetylneuraminic acid aldolase. **Jason Porta**, U. Nebraska Med. Ctr., discussed the development of a technique to utilize first-order satellite reflections in examining low-resolution actin filament formation. **Brandon Mercado**, UC Davis, presented new structures of metalofullerene cages and discussed problems in determining these structures. **Greg A. Hogan**, U. Missouri-St. Louis, talked about several crystal structures of small molecules trapped in an ordered metal-organic framework. **Julie Aaron**, U. Penn., showed the crystal structure of epi-isozizanene synthase, a class I terpene synthase, in a "closed-liganded" and "closed-unliganded" form. The loss of the ligand in the closed-unliganded form caused a large conformational change. **Gina Thede**, U. Alberta, and her colleagues have been working on the CpxP protein, a repressor of the Cpx pathway that senses mis-folded proteins. They used multi-angle laser light scattering to show that CpxP is a dimer both at pH 5.8 and pH 8.0; this was confirmed by SAXS and cross-linking. Finally, **Arbin Rajbanshi,** Kansas State U., presented structures of auto-assembling hydrogen and halogen-bonded capsules. He discussed the potential use of these cavitands in encapsulating and transporting small molecules.

Svilen Bobev, left, accepting the Etter Early Career Award from ACA president Bob Von Dreele. Photo by Peter Müller.

Bobby Heuther, at right, presenting the YSSIG Etter Student Lecturer Award to Ivan Campeotto.

Robert Huether

Editor's note: Other plenary lectures were: the Buerger Award lecture by Michael James (see SP05 report on opposite page; the Warren Award lecture by Shih-Lin Chang, a somewhat edited version of which will be in the spring, 2010 ACA RefleXions; the Etter Early Career Award lecture by Svilen Bobev, see above; and, opposite page, Ted Baker's "Celebrating Crystallography." .

Ted Baker with his Structural Biology group at the University of Auckland. Photo from Ted's U. Auckland website.

SP.03: Celebrating Crystallography

Ted Baker's fine historical lecture began by citing Louis Pasteur who provided one of the most important demonstrations of the idea that external form must reflect internal structure, an idea that crystallographers have enthusiastically adopted and applied to the elucidation of atomic and molecular structures. His talk featured pioneers in crystallography: William and Lawrence Bragg, Dorothy Hodgkin, J. D. Bernal, Linus Pauling, Max Perutz, and Francis Crick were superb examples of those who have tackled the mysteries of chemistry and biology. He concluded with the idea that atomic structure has connections with biology, chemistry, mathematics and even art and architecture.

Ted, a past-president of the IUCr, leads a group (pictured above) of more than 40 researchers at the University of Auckland. He directs the Maurice Wilkins Centre of Molecular Biodiscovery, one of seven New Zealand National Centres of Research Excellence.

SP.05: Buerger Award Plenary Lecture by Michael James

From Sillimanite to Structural Biology or from Minerals to Macromolecules was the title of the story told by **Michael James**, the recipient of the **2009 Martin J.Buerger Award**. Michael took his audience on a very enjoyable time travel session, from his early "exposure" to x-rays at the University of Manitoba via his doctoral studies with Dorothy Hodgkin at Oxford to his long-lasting appointment at the University of Alberta. The slides that accompanied his talk stretched from beautiful precious stones (Michael expressed regret that he did not save all the samples) and snapshots taken at a number of historic occasions (e.g. David Phillips' public lecture presenting the structure of lysozyme) to the first protein structures determined in Canada (*Streptomyces griseus* protease and penicillopepsin) -before touching on a few examples from the rich selection of macromolecular crystal structures, especially those of members of the other families of proteolytic enzymes, protease inhibitors, $Ca2^{+}$-binding proteins and -not to be forgotten- ß-lactamases. He then concentrated on his present research focus, the crystal structures of proteins that form the biosynthetic pathways for arginine and methionine in *Mycobacterium tuberculosis*. Active and productive as ever, Michael is looking forward to adding many more entries to his laboratory's long list of successes.

Michael James, at left, receiving the award from ACA President, Bob von Dreele. Photo by Peter Müller.

Emil Pai

Contributors to this issue

Christer Aakeröy, Marc Allaire, Ross Angel, Eddy Arnold, Christine Beavers, Jim Britten, Jim Browning, Sue Byram, Wah Chiu, Patti Coley, Ed Collins, Marcia Colquhoun, Philip Coppens, Jean-François Couture, Jamaine Davis, Bill Duax, Caroline Duax, Gary Enright, Steven Evans, Bill Furey, Ovidiu Garlea, Peter Gehring, Ilia Guzei, Marvin Hackert, Peter Horanyi, John Horton, Bobby Huether, Ashfia Huq, Ryan Jackson, Christopher Kimberlin, Herb Klei, Tom Koetzle, Tad Koga, Peter Kwong, Eric Lawrence, Byeongdu Lee, Cora Lind, Kristin Low, Colin McCrimmon, Alex McPherson, Duncan McRee, Pierangelo Metrangelo, Jinrong Min, John Mitchell, Peter Müller, Ken Ng, Joe Ng, Craig Ogata, Emil Pai, Matt Peterson, Gil Privé, David Rose, Bernhard Rupp, Bernie Santarsiero, Dmitriy Soldatov, Richard Staples, Jack Tanner, Iris Torriani, Crystal Towns, Hiro Tsuruto, Tim Umland, Felix Vajdos, Britt Vandhura, Bob von Dreele, Xiaoping Wang, Mark Warren, Thomas Weiss, Pamela Whitfield, Carrie Wilmot, Ian Wilson, Joyce Wong, Victor Young, Bomina Yu.

TR01 pm l to r: Michael Ruf, Diego Gatta, Thomas Proffen, Mathias Meyer, Ian Swainson, David Brown, Ross Angel, Michal Dusek.

TR.01: ACA Transactions Symposium on Phase Transitions

Phase transitions, in which a structure changes from one atomic arrangement to another without a change in composition, provide the most rigorous arena for testing ideas about the forces and balances of forces that stabilize particular atomic configurations in crystal structures. The study of phase transitions has direct applications in pharmacology and drug design where the issue of stable polymorphs is critical, and most modern materials used in devices (gmr materials, piezo- and ferro-electrics and multi-ferroics) derive their technological properties from structural phase transitions. While the study of phase transitions has previously been a major focus of solid state physics and mineralogy, the advent of fast and accurate area detector technologies together with reliable and automated temperature control systems, means that the study of phase transitions in molecular systems can become routine provided the methods of analysis are known. In the 2009 *Transactions* Symposium, a broad selection of the concepts and characterization techniques developed for studying phase transitions were presented.

Simon Parsons, U. Edinburgh, used the example of his work on the high-pressure polymorphism of salicylaldoxime and of serine to demonstrate that while phase transitions sometimes appear to be driven by bonding forces, such as H-bonds being forced to become short, the dominant factor in determining polymorph stability at high-pressures is the packing efficiency. The pressures involved, of several GPa, mean that the PV term becomes the dominant component of the free energy of a molecular crystal. The same conclusion was drawn by **Diego Gatta**, U. Milan, in his wide-ranging review of the behavior of zeolites at high pressures. The general response of zeolites to increasing pressure is one of continuous rotations of the tetrahedral units comprising the framework, and relatively rare transitions occur through the same rotations in a discontinuous way, so that the volume is greatly decreased. **I. David Brown**, McMaster U., summarized the essential message in the context of an exploration of bonding forces through the concept of bond valence. David emphasized once again that chemistry does not change between phases or across phase boundaries, but that phase transitions are driven by changes in the intensive external thermodynamic variables such as temperature or pressure.

Structural phase transitions are a special class of transitions in which the symmetries of the two phases have a group-subgroup relationship, and the lower-symmetry structure can be regarded as a distorted version of the high-symmetry form. The power of analyzing structural phase transitions from a group-theoretical point, and the resulting structures, was emphasized in two presentations. **Branton Campbell**, Brigham Young U., showed that the apparently complex structural evolution of the distorted low-symmetry phase below a transition can often be more simply and naturally explained in terms of "symmetry-adapted distortion modes" which he called "Nature's basis for parameterizing structural phase transitions". The essence of a distortion can often be captured by a relatively small number of the available modes, while the other modes have amplitudes that cluster near zero. As a consequence, the symmetry-adapted description reduces the effective complexity, leading to a clearer understanding and more stable refinement of crystal structures to diffraction data. Close to high-temperature phase transitions such modes can represent the dynamic fluctuations of the structure. **Thomas Proffen**, LANL, reported that, by analyzing the total scattering in terms of a probability density function, one can show that many displacive transitions in oxides involve no change in local structure but merely a change in the long-range correlations. **Manuel Perez-Mato**, U. del País Vasco, extended the symmetry-mode approach to the analysis of phase transitions that give rise to multi-ferroic materials. He emphasized the power of Landau theory and introduced the concept of symmetry-adapted order parameters (equivalent to mode amplitudes), to couple the macroscopic thermodynamics of the low-symmetry phase directly to the microscopic distortions of its atomic structure.

One session of the symposium was devoted to presentations of software tools that help in the processing and refinement of the more complex diffraction data that arises from crystals that have undergone phase transitions. **Mathias Meyer**, Oxford Diffraction, demonstrated that indexing and integrating diffraction patterns from crystals that have become twinned as a result of a phase transition is straightforward with the tools now available; **Michel Ruf,** Bruker-AXS, showed

TR01, Transactions, cont'd

the same is true for the integration of diffraction patterns from incommensurately modulated crystals; and **Michel Dusek**, Inst. Physics, ASCR, Prague, demonstrated the power of the Jana software for determining and refining both twinned and modulated structures.

The 2010 ACA meeting in Chicago will feature a session devoted to the study of the mechanisms of phase transitions.

Ross J. Angel

TR01 am l to r: Kenneth Haller, Chae Un Kim, Branton Campbell, Ross Angel, Manuel Perez-Mato, Simon Parsons

"Reflections" photos of downtown Toronto by Peter Müller.

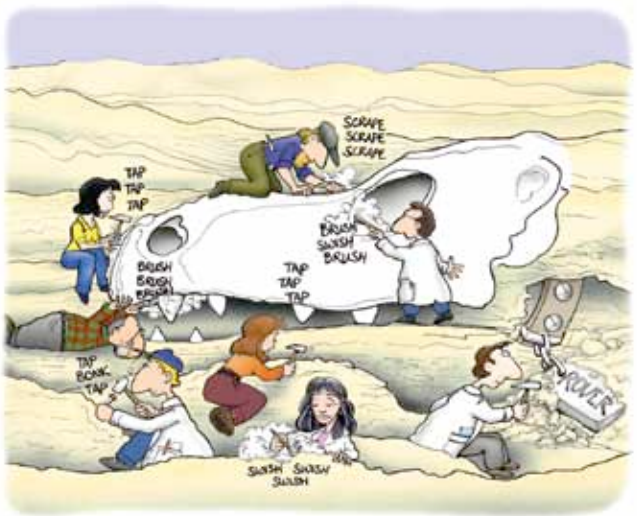
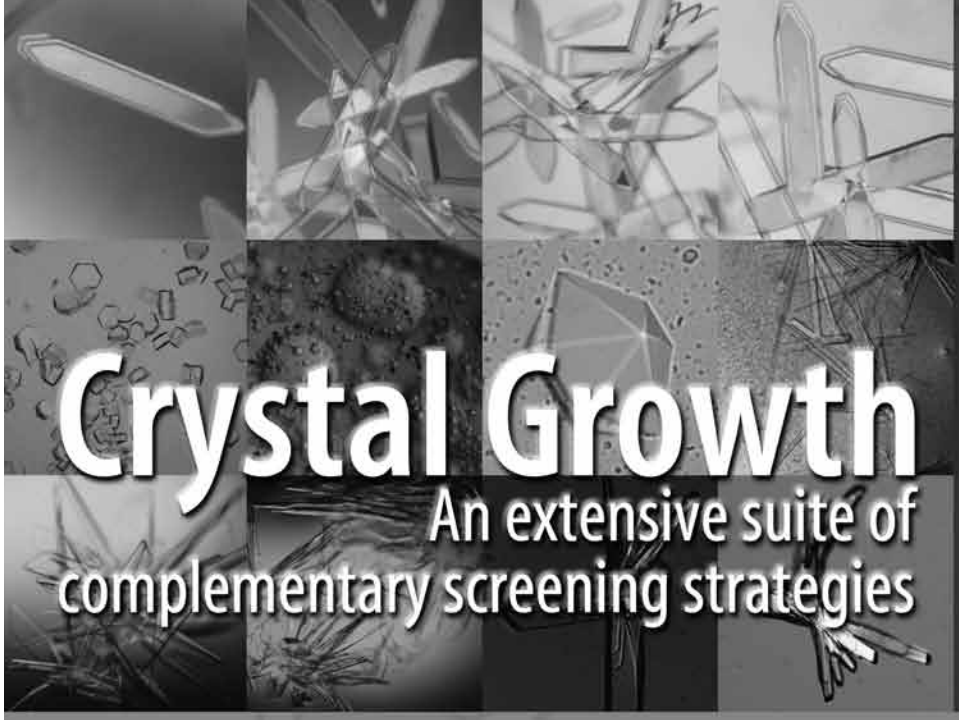


Photo courtesy of Nick D. Kim, nearing-zero.net.



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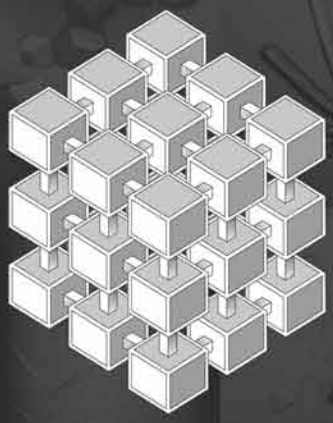

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1.02: Vaccine Design

l to r: Ian Wilson, Bing Chen, Brian Baker, Peter Kwong, William Schief, Rino Rappuoli.

Three talks highlighted the application of vaccines to viruses, bacteria and cancer. **Ian Wilson**. Scripps, described broadly neutralizing antibodies against influenza virus hemagglutinin. Most antibodies elicited against hemagglutinin are strain specific, and current vaccines need to be taken seasonally. Ian highlighted the structural characterization of new antibodies, which recognize a conserved stem epitope. The identification of these more broadly neutralizing antibodies suggests the potential for a more universal flu vaccine, effective not only against the seasonal flu strains, but also against larger antigenic jumps, which occur less frequently, but have the potential to generate global pandemics with mortalities in the 10s of millions.

Brian Baker, Notre Dame, then discussed Cytotoxic T cells, which recognize T cell epitopes in the context of MHC-I. Structures of T cell epitopes, T cell receptors and MHC-I ternary complexes were reviewed to provide an appropriate structural context. Manipulation of anchor residues within weakly bound T cell epitopes to attain higher stability with MHC-I has been shown to improve cytotoxic effects, and Baker presented his findings on melanoma antigens recognized by T cells. Structural characterization of anchor residue changes for 9-mers and 10-mers in complex with MHC showed only minor structural changes, despite large differences in biological outcomes. Differences in epitope flexibility might possibly explain this perplexing finding, but it is evident that there is a gap in current understanding. How do crystal structures of MHC-I with peptide antigens relate to actual cytotoxic effects, and how does one design antigens to combat cancer?

Rino Rappuoli, Novartis, started with a history of the technological revolutions affecting vaccine development, from the landmark Pasteur methodologies, to glycoconjugates and recombinant DNA techniques in the 1980s, to genomic techniques in the 1990s and 2000's, ending with the prediction that structural biology would enable yet another revolution. Progress with meningococcal disease is just such a present day revolution, with effective vaccines developed against types A, C, W and Y of meningococcus with glycoconjugates, and against type B with genomic techniques leading to the current Phase III vaccine comprising 5 different genomically identified proteins. Structural analysis of one of these bacterial proteins, the factor H binding protein, showed how this protein binds factor H and prevents C3 lysis. Antibodies which recognize the factor H binding protein cause bacterial lysis, although this occurs in a strain-specific manner. The combination of structural, sequence, and antigenic information enabled the creation of chimeric factor H binding proteins, which elicit antibodies effective against diverse meningococcus B.

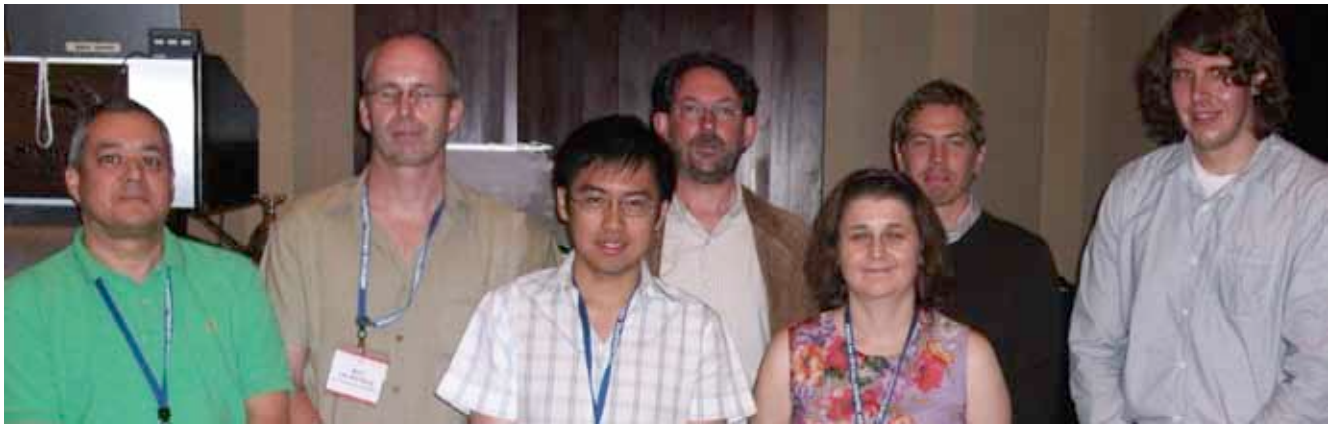
Three talks on HIV-1 vaccine development highlighted diverse ways in which structural biology can enhance the different and challenging stages of vaccine development, from epitope identification, to immunogen design and even to vaccine delivery. **Bing Chen**, Harvard, began by describing recombinant adenovirus, a central player in the delivery of vaccine antigens. Unfortunately, one of the most potentially useful strains of adenovirus, AD5. suffers from pre-existing immunity in a significant fraction of the human population. Structure-based engineering of the adenovirus hexon, with the transplantation of the 7 hexon hypervariable loops from a rare adenovirus serotype (Ad48) to Ad5, resulted in a new chimeric virus which retained most of the useful Ad5 properties with respect to vaccine delivery, but antigenically resembled the rare Ad48 serotype. Chen followed this with an in depth description of the HIV-1 envelope glycoproteins (gp120 and gp41), especially their role in viral entry and the conformational changes they undergo from prefusion, to prehairpin intermediate, to post-fusion states. Engineered proteins designed to mimic the HIV-1 envelope glycoproteins in each of these states were described, with focus on a mimic of the prehairpin intermediate which has enhanced affinity for the broadly neutralizing antibodies 2F5 and 4E10.

Bill Schief, U. Washington, reported on his application of computational design to "re-elicit" neutralizing antibodies. The program *Rosetta* is a proven design platform developed by David Baker and colleagues. Schief described his new methods: *side-chain grafting* and *backbone-grafting* which utilize *Rosetta* to transplant linear epitopes - defined crystallographically in complexes with broadly neutralizing antibodies - to proteins in the PDB. These epitope scaffolds can be use in combination or in series (prime-boost) to focus the immune response on the desired epitope. Examples of work in progress with epitope scaffolds containing linear epitopes for 2F5, as well as for 4E10, were presented.

Peter Kwong, Vaccine Research Center, NIH, presented concepts from Dennis Burton and other IAVI (International AIDS Vaccine Initiative) colleagues that explain how broadly neutralizing antibodies against HIV-1, identified from HIV-1 infected individuals, might be used in vaccine development. A process of retrovaccinology was outlined, whereby the broadly neutralizing antibody is defined at the atomic level in complex with bound epitope. Then, working backwards from the epitope definition, one might design an immunogen capable of eliciting the desired broadly neutralizing antibody. Because monoclonal and phage display techniques may identify unusual antibodies, not readily elicited in any quantities in vivo, the prevalence of such antibodies - naturally elic- *cont'd, next page*

1.02, cont'd ited in HIV-1 infected individuals - may be a useful consideration. Evidence was presented that 2F5- and 4E10-like antibodies are rarely elicited in natural infection with HIV-1, whereas the b12 antibody, which targets a complex epitope involving a subset of the binding site on gp120 for the CD4 receptor, appeared to be more frequently elicited. An ideal immunogen to elicit b12-like antibodies might be one with high affinity for antibody b12 and antigenic specificity for only b12-like antibodies. Structure-based techniques to increase antigenic specificity such as antigenic substitution, conformational stabilization, and glycan or PEG silencing were described.

Ian Wilson & Peter Kwong



L to r: Bernie Santasiero, Bert van den Berg, Peter Chan, Paul Adams, Carrie Wilmot, Peder Cedervall, and Brandon Goblirsch.

1.04 Green Biochemistry

This session was organized to focus on research relating the production of biomass, carbon neutral biofuels, bioremediation, and biocatalysis. Structural biology will play a significant role in the study of the mechanism and modification of enzymes from microbial and plant systems.

Paul Adams, LBL, discussed some of the research being carried out at the Joint BioEnergy Institute at Lawrence Berkeley Lab. The goal is to produce higher yielding crops of plant materials as high-energy sources at a low cost. This involves the study of energy conversion where plants use carbon dioxide and water to eventually burn as carbon dioxide and water, and to study the decomposition of cell wall components.

Bert van den Berg, U.Mass. Medical School, presented some of his results on bioremediation and biodegradation studies with Gram negative bacteria. Two major transport mechanisms were evaluated for the membrane-associated proteins TodX and TbuX using site-directed mutants.

Three student presentations followed, and focused on structural and mechanistic studies of enzymes involved in bioremediation. **Brandon Goblirsch**, U. Minnesota, focused on chlorite dismutase, Cld, with the ultimate goal of removing perchlorate from the environment. There were substantial differences when comparing Cld between different organisms. **Peter Chan**, U. Toronto, reported on his research involving a dehalogenase, in an effort to remove fluorinated organic molecules from the environment. Peter used site-directed mutagenesis and kinetic parameters to identify key residues in the reaction. Finally, **Peder Cedervall**, U. Minnesota presented his structural results on an enzyme involved in the methanogenesis pathway for the microbial generation of methane. Methyl-coenzyme M reductase has an active site containing a Ni-porphyrin that binds carbon dioxide or methanol. These types of enzymes are important in the generation of energy-rich biosources, like methane.

Bernie Santarsiero & Carrie Wilmot

l to r: Jian Xu, William Price, Alex McPherson, Irimpan Mathews, Aiping Dong, Ilana Goldberg, Zygmunt Derewenda, Bernhard Rupp, Nadrian Seeman, Nicoleta Economou.

1.03: Crystallization Methods

The early portion of the session was devoted to macromolecular crystallization, with the implicit acknowledgement that "your protein is your most important parameter". The practicalities of using this realization were discussed by the first three speakers.

In an introductory talk **Bernhard Rupp**, Q.E.D. Life Sciences, addressed the question, what have we learned from high throughput protein crystallography initiatives with regard to its value to the practitioner in his individual, often "not-so-high throughput" research? Because each individual protein determines, by its inherent properties, the outcome of a crystallization experiment, many challenges remain for the analysis and prediction of crystallization properties. Repeatedly it has been demonstrated that modifying an obstinate protein is a more promising path to crystallization than additional screening. However, the causal relation between targeted changes and subsequent crystallization success is in many cases hard to establish. Bernard emphasized that developing novel means of expressing – in sufficiently soluble form - and crystallizing difficult mammalian proteins, protein complexes, and membrane proteins remains a formidable challenge to crystallographers.

Zigmunt Derewenda, U. Virginia, began by questioning a decade or so old dogma that crystal contacts in protein crystals are stochastic in nature. Data was presented showing that in a data base of 800+ strictly monomeric proteins, the crystal contacts were clearly enriched in small, hydrophobic residues, while depleted in large, polar amino acids. It was further demonstrated that side chain entropy is the principal property that negatively correlates with crystal-contact forming propensity. A server has been designed for automatic prediction of such sites based only upon sequence. Zigmundt's conclusion was that protein surface engineering can be used in a rational fashion to obtain crystals of proteins otherwise recalcitrant to crystallization, or to generate crystals with superior diffraction properties.

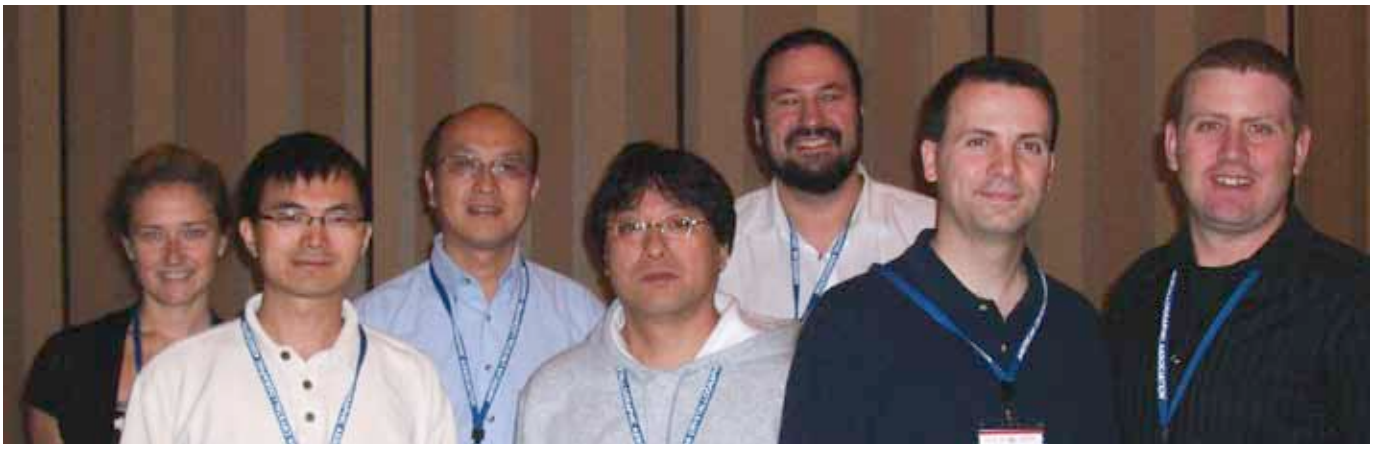
Bill Price, Columbia, presented an analysis of some of the physical properties of proteins, (as can be judged from their amino acid sequences), that most strongly correlate with two practical aspects of structural biology: protein solubility and crystallization propensity. Based on the results of thousands of experiments conducted by the NSGC, it was found that sequences positively correlating with solubility are the same sequences that negatively correlate with crystallization propensity. The findings appear to place protein crystallographers, once again, squarely between a rock and a hard place.

Practical aspects of crystallization and the preparation and manipulation of crystals for data collection were addressed next. **Aiping Dong**, U. Toronto, presented experimental results from Aled Edwards' group showing that in numerous cases proteins that otherwise failed to crystallize would do so after exposure to proteases. Structural analyses showed that the proteins were invariably trimmed of flexible loops and loose ends. **Ilana Goldberg**, Georgetown U., described experiments and some initial data on the use of two-dimensional surfaces of designed chemical features to promote the nucleation of crystals. **Irimpan Mathews**, Stanford, addressed the problem of mounting small and fragile crystals for analysis and presented results demonstrating the value of *in situ* data collection. In his experiments he grew crystals in cryo loops thereby making direct freezing and data collection possible without investigator intervention.

Nicoleta Economou, Drexel U., described the use of proteins as crystallization chaperones for "large" small molecules, such as glycopeptide antibiotics. The thiol-based chemistry is applicable, however, not only to conventional molecules, but to other proteins as well. **Jian Xu** described a fluorescence based optical system that uses the inherent fluorescence of aromatic residues. With this system, it was possible to identify small protein crystals, even when accompanied by heavy precipitate, and to discriminate protein crystals from salts and small molecules.

A highlight of the session was a *tour de force* presentation by **Ned Seeman**, New York U., who described the synthesis, construction, and x-ray diffraction analysis of "designer" DNA crystals. Representing more than thirty years of research and development, his presentation was truly remarkable. His approach opens up possibilities for delineating the structural and dynamic properties of DNA as a function of a whole host of physical and chemical variables. Furthermore, the use of such crystals holds great promise for the development of ligands and drugs that interact specifically with defined sequences of DNA.

Alex McPherson



l to r: Melanie Adams-Cioaba, Jinrong Min, Rui-Ming Xu, Toshiya Senda, John Horton, Raymond Trievel, Jean-François Couture.

1.05 Chromatin Remodeling

Several novel protein structures were presented that should open new avenues of thought about the mechanisms controlling the post-translational modifications of histone proteins.

Raymond Trievel, U. Michigan, reported on lysine biosynthesis from a fungal homocitrate synthase. His talk emphasized the biological interplay between dimerization and enzymatic activity of the enzyme. By combining crystallographic data and *in vivo* experimentation, he provided insights about what could be a novel and unique target for drug design to aid immunodepleted patients suffering from mycosial diseases.

The next two talks took on fundamental questions about chromatin biology. The structural bases underlying the stimulatory role of histone or other covalent post-translational modifications were discussed; also allosteric regulation of chromatin-modifying enzymes; the deposition of histones onto DNA; and the recognition of histone methyl marks. **John Horton**, Emory, reported on new structures of two related human demethylases, each of which contains a plant homeodomain (PHD) that recognizes the trimethylated lysine, and a jumongi domain that can catalyze demethylation. This a significant step towards understanding how histone methyltransferases and demethylases work; also, they are the first structures exhibiting a bona fide *trans/cis* mechanism for a histone modifying enzyme. **Rui-Ming Xu**, Chinese Academy of Sciences; National Laboratory of Protein Science, a pioneer in the field, reported on the co-crystal structure of Sir2/Sir4; the structure provides a basis for the observation that the binding of Sir4 greatly increases the histone deacetylase activity of Sir2.

Next, **Toshiya Senda**, Japan Biological Information Research Centre, provided biochemical evidence that the histone chaperone CIA could interact with histone and bromodomain-containing proteins by using distinct binding modes; and **Melanie Adams-Cioaba**, U.Toronto, presented the structure of the Fragile X Mental Retardation Protein 2 double Tudor domain. These two talks, although they were not mechanistically or functionally related, elegantly illustrated the diversity of histone binding modes that the cell has devised to translate histone modifications into biological signals. In a related poster, **Paul del Rizzo**, U. Michigan, presented his work on the histone H3 Lys-4 methyltransferase SET7/9. Combining crystallographic and biochemical experiments, del Rizzo identified key SET7/9 active site residues that control the addition of one, two or three methyl groups to its substrate lysyl side chain. Considering that the degree of lysine methylation plays an important role in a plethora of biological processes, the del Rizzo data may provide information about the role that different degrees of methylation provide genome-wide.

Jean-François Couture Couture and Jinrong Min

L to r: Eugene Masters, Jeff Abramson, David Rose, Lyann Sim, Xiaoqiang Wang, Anne Imberty, Mark Currie, Ian Schoenhofen, Ken Ng.

1.06: Carbohydrate Recognition

Structural studies on carbohydrate recognition have led to key insights in a wide range of biological processes, including microbial pathogenesis, energy metabolism, immune recognition and secondary metabolism.

Anne Imberty, CNRS, France, outlined beautifully her studies investigating the structural and biochemical basis of fucose and mannose recognition in lectins from *Pseudomonas aeruginosa* and other bacterial pathogens. It was encouraging to see how this work progressed from basic crystallographic and thermodynamic studies towards advances in the design of multivalent carbohydrate mimetics. These may ultimately become novel therapeutics for common diseases such as cystic fibrosis. **Jeff Abramson**, UCLA, presented the crystal structure of a sodium galactose transporter, which is the first structurally characterized member of the SSS family (solute sodium symporters). Fourteen transmembrane helical segments form a large aqueous cavity that is observed in the 'inward occluded' conformation holding a single galactose molecule shielded from the outside by hydrophobic residues. Unexpectedly, the protein shows an inverted topology repeat. In the first portion of his talk Jeff gave a fascinating and entertaining description of how they had systematically improved the quality of their crystals from about 8Å to about 3 Å resolution. **Lyann Sim**, U. Toronto, presented the structural basis for the differential substrate specificities of human maltase-glucoamylase and sucrase-isomaltase SI in terminal starch digestion. She showed how these high-resolution determinations could advance the development of specific inhibitors to control blood glucose levels in type II diabetes. **Xiaoqiang Wang**, Noble Foundation, described the 2.1 Å structure of the glycosyltransferase UGT78G1 from *Medicago truncatula*, which provided interesting insights into possible enzyme-catalyzed deglycosylation.

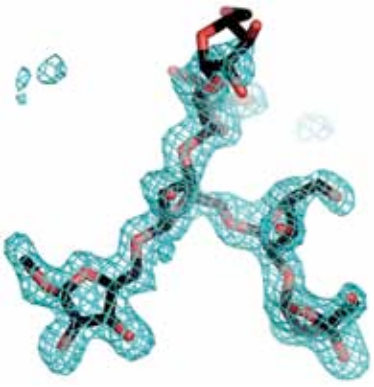
David Rose, U. Waterloo/ U. Toronto, summarized recent results from the extensive studies that his group has made into the recognition of substrates and inhibitors of α-mannosidase II, which has been identified as a target for inhibition of glycosylation in cancer metastasis and microbial infection. David showed for the first time the complex with the full hepta-saccharide, as well as new structures with analogues of the natural inhibitor swainsonine that reveal its potential as a therapeutic.

Eugene Masters, Southern Research Institute, presented novel structures of *Mycobacterium tuberculosis* ribokinase in complex with ribose and AMP-PNP, revealing an intriguing asymmetric dimer that may be of importance to catalysis and regulation.

The first structure of an ADP-dependent phosphofructokinase, which adopts a fold very similar to ribokinase, was described by **Mark Currie**, Queen's U. Mark described the elegant combination of structural analysis and site-directed mutagenesis which was used to identify key residues involved in substrate recognition. Finally, **Ian Schoenhofen**, NRC, presented the first structure of a metal-independent NDP-sugar hydrolase from *Campylobacter*, PseG, an enzyme required for pseudaminic acid biosynthesis and protein glycosylation. A combination of careful structural analysis and mutagenesis were used to deduce a mechanism of catalysis that shows surprising similarity to the MurG glycosyltransferase.

A related poster byTomohiko Murase, U. Calgary, is shown below.

Steven Evans and Ken Ng



An image from the PM49 poster by Tomohiko Murase and coworkers. The figure shows the model of an arabinofuranoside hexasaccharide bound to the Fab fragment of the CS-35 monoclonal antibody superimposed on an omit electron density map calculated with data extending to 2.0Å resolution. This is the first structure of an oligofuranoside-protein complex and also the first structure of a portion of the lipoarabinomannan polysaccharide from mycobacteria. The work was recently published electronically in JMB (doi:10.1016/j.jmb.2009.06.074).

L to r: Roger Durst, Matt Peterson, Francisco Hernandez-Guzman, Pierre Le Magueres, Douglas Davies, Bruce Noll, Ray Scaringe.

3.01: New Technology in Industry

A diverse series of talks included the use of fragment based drug discovery by **Doug Davies**, deCODE Biostructures; automated small molecule structure determination for benchtop diffratometers, by **Bruce Noll**, Bruker-AXS; new developments in monochromator technology by **Roger Durst**, Bruker-AXS; and a new collection of Pipeline Pilot protocols for macromolecular refinements by **Francisco Hernandez-Guzman**, Accelrys.

Ray Scaringe, Bristol-Myers Squibb, used statistical analysis of Bijvoet differences to determine the absolute structure of small compounds containing only C, H and N atoms. The absolute structures of all seven examples shown were unambiguously determined. Ray pointed out that these methods can be applied very early in the pharmaceutical process to help medicinal chemists make informed decisions about the compounds they are advancing.

Pierre Le Magueres, Rigaku, reported that the effects of UV irradiation, (using LEDs in multiwell crystallization plates), on the stability of protein crystals depends on the exposure time. In the particular proteins discussed it was clear that typical exposures during imaging had no immediate effect on the structures. More prolonged exposures did cause some changes in structure. The discussion that followed made it clear that concerns remain about the general idea of exposing proteins to the UV radiation used in imaging systems, but only time and practice will tell when special precautions are necessary.

Matt Peterson

L to r: Tad Koga, Peter Gin, Juergen Kraeusslich, Ming Hwa Kim, Hiroshi Jinnai, Eugenia Kharlampieva, Aleksandar Kremenovic, Jim Browning, Ting Xu, Byeongdu Lee.

4.01: Characterization of Nanomaterials

The speakers in this session described the formation, transformation, and property of nanostructures.

Hiroshi Jinnai, Kyoto Inst. Tech., talked about their novel methodology for characterizing nanoscale structures of block copolymers by combining transmission electron microtomography (TEMT) and neutron reflectivity (NR). Hiroshi has recently established TEMT which provides three-dimensional images of structures at nm resolution and applied it to a variety of soft matter systems including polymer blends, block copolymers, microemulsions, and polymer nanocomposites. He described how real space and reciprocal space analysis can be complementary in nanostrucuture characterization.

Peter Gin, SUNY Stony Brook, the recipient of the SAS SIG **2009 Etter Student Lecturer Award** presented current research on the anomalous swelling of polymer thin films induced by density fluctuations in supercritical carbon dioxide ($scCO_2$). The utilization of $scCO_2$ is touted as a "green" alternative to the conventional techniques that use toxic organic solvents. Peter and his colleagues established a new method that facilitates enhanced swelling, - as much as 30-60 % in a wide variety of polymer thin films, specifically when the bulk polymers have very poor miscibility with CO_2. They focused on "CO_2-philic" polymers to determine the role of inherent miscibility on the extent of excess swelling in polymer thin films. Using *in situ* neutron reflectivity, they showed that excess swelling is a general phenomenon regardless of the inherent miscibility with $scCO_2$.

Ting Xu, UC Berkeley, talked about block copolymer (BCP)-based supramolecules constructed by associating small molecules to the side chain of one block, forming coil-comb shaped supramolecules. Upon phase separation, the small molecules provide rich chemical functionalities and molecular level assemblies and diblock copolymers may manipulate their assembly macroscopically as well as for easy processing. The hierarchical assemblies of supramolecules, consisting of polystyrene-b-poly(4-vinylpyridine), or PS-b-P4VP, with 3-pentadecylphenols (PDP) hydrogen-bonded to 4VP, were investigated after solvent annealing in a chloroform atmosphere. The synergistic co-assembly of PS-b-P4VP and PDP was used to generate oriented hierarchical structures within thin films. Hierarchical assemblies including lamellae-within-lamellae and cylinders-within-lamellae were simultaneously ordered and oriented from a few to several tens of nanometers over a macroscopic length scale. She showed that the macroscopic orientation of supramolecular assembly depends on the comb block fraction and can be tailored by varying PDP to 4VP ratio without interfering with the supramolecular morphologies.

Eugenia Kharlampieva, Georgia Inst. Tech., discussed the structure and properties of polyelectrolyte layer-by-layer (LbL) films. The internal structure of two related classes of LbL films, where interactions between adjacent layers are controlled by either hydrogen-bonding or electrostatic forces, was probed by neutron reflectivity. The degree of interpenetration of polymer layers was found to be strongly correlated with the strength of intermolecular interactions between the adjacent layers. A combination of spin assisted assembly (SA) with LbL made the films more stratified, with strongly pronounced layering as compared to conventional LbL films. In addition, the degree of interpenetration in SA multilayers expressed as the interlayer roughness was controlled by the salt concentrations of the solutions used for the deposition. Eugenia reported that structural information about such films, as well as control over multilayer internal organization, is crucial to optimizing their performance.

Myung Kim, UCSB, presented new nanowire growth mechanisms studied by *in-situ* grazing incidence small angle x-ray scattering (GISAXS). Nanometer size liquid droplets formed at temperatures below the bulk melting point become supercooled as they grow through Ostwald ripening and can be exploited to grow nanowires and nanorods. Myung and his colleagues used this approach to synthesize a number of highly crystalline metal oxide nanowires in a chemical vapor deposition furnace. They observed dramatic changes in nanowire growth when substrates were varied, reflecting the influence of wetting forces on supercooled nanodroplet shape and mobility.

Tad Koga, Byeongdu Lee, and Jim Browning

Philip Coppens talking with Angela Criswell.

5.01: Cool Structures

l to r: Joseph Tanski, Peter Müller, Edwin Stevens, Juan van der Maelen, Nobuhiro Mizuno. Photo taken with Peter Müller's camera.

"Cool" was interpreted by all speakers as crystallographically interesting.

Ed Stevens, U. of New Orleans, discussed his crystal structure of an α-trehalose dihydrate, a non-reducing disaccharide in which the glycosidic oxygen atom is shared by the anomeric carbon atoms of each of the two glucose rings. Ed used a combination of classical and charge density methods, theoretical calculations and various spectroscopic methods to examine the exo-anomeric effect.

Nobuhiro Mizuno, SPring-8, presented his charge densitiy (synchrotron x-ray) and nuclear density (neutron diffraction) studies of rare-earth/transition-metal hydride clusters. Mizuno used maximum entropy methods on both sets of data; the complementary information enabled him to directly visualize hydrogen behavior and thus explore correlations between structure and property of multimetallic polyhydride clusters.

Joe Tanski, Vassar, reported on his *adventures in coordination chemistry with bad ligands*. Among the unwanted compounds in his crystal structures (often decomposition products or starting materials), were several interesting structures of metal precursors cocrystallized with uncoordinated ligands.

Juan van der Maelen, U. of Oviedo, brought the focus back to charge density methods. Comparing results from multipole refinement of the experimental electron densities and their topological analyses by means of R.F.W. Bader's *Atoms in Molecules* theory with theoretical *ab initio* calculations, van der Maelen asked the question "is there any real bond between metal atoms in the clusters $[Zn_2(\eta^5\text{-}C_5Me_5)_2]$ and $[Ru_3(\mu\text{-}H)_2(\mu 3\text{-}MeImCH)(CO)_9]$?"

Peter Müller

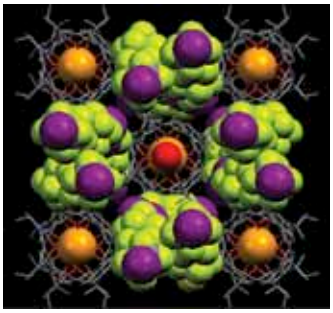
6.01 Supramolecular Chemistry

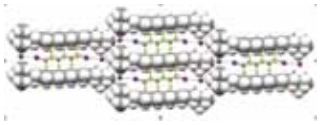
l to r: Menahem Kaftory, Dejan-Kresimir Bucar, Dmitriy Soldatov, Gautam Desiraju, Pierangelo Metrangolo.

Despite the odors produced by the garbage strike that happened to be running in parallel with the ACA meeting in Toronto, there was a sweet smell of success about this symposium. Twenty-three speakers from seven nations presented work on intermolecular forces, non-covalent assembly, crystal growth, materials design, pharmaceuticals, and database studies. Appropriately, 20 years after the appearance of his seminal book on crystal engineering, **Gautam Desiraju**, Indian Inst. of Science, was first to speak. He offered an insightful look at polymorphism and at structures with high Z' numbers, as well as a spirited (and enjoyably provocative) defense of the importance and relevance of small-molecule crystallography.

Pierangelo Metrangolo, Politecnico de Milano, gave a clear and educational description of halogen bonding, an interaction that is non-covalent. Metrangolo also presented his recent work on ways that halogen bonds can be used to separate perfluorinated alkanes. See images below and at right.

A view down the c axis of the crystal structure of the supramolecular complex formed by 4-tert-butylcalix[4]arenetetra-N, N-diethylacetamide, BaI_2, and 1,8-diiodoperfluorooctane. Ba orange, I purple, F green, O red, N blue, C gray. The calixarene molecules are represented by capped sticks, and all other components by van der Waals spheres. Hydrogen atoms are omitted for clarity. In this homochiral supramolecular complex, the perfluorinated modules exclusively adopt a right-handed (P) helical conformation (molecular chirality), which translates into chiral and enantiopure fluorous double helices (supramolecular chirality), owing to strong and directional I···I-C halogen bonding. Angew. Chem. Int. Ed. 2006, 45, 1915.

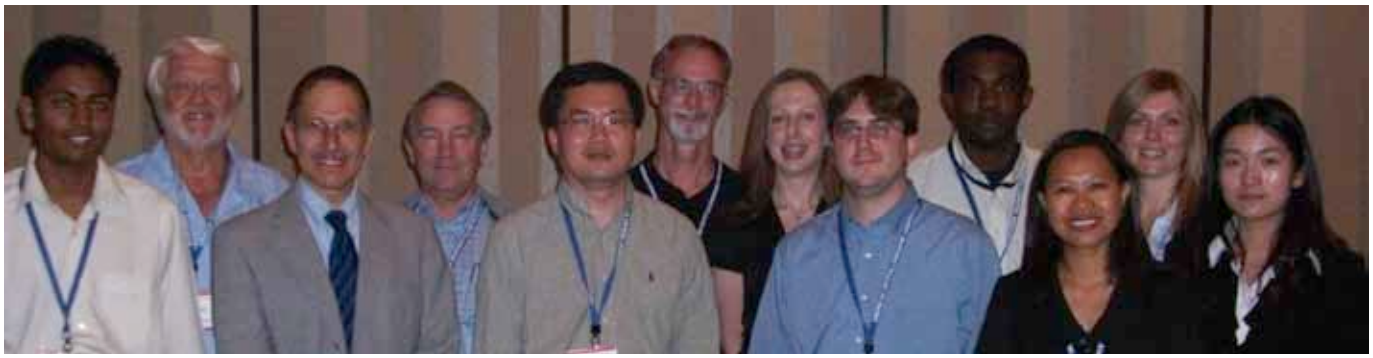




The complex dodecamethonium iodide/diiodoperfluorohexane 1c·2c viewed along the a axis. Four HC cations define a rectangular parallelepiped, i.e. a molecular container, topped with two I- ions, in the well-defined cavity of which the DIPFA 2c is trapped due to the strong XB to the two I- ions.

At right, l to r: Alicia Beatty, Safiyyah Forbes, James Wuest, Heba Abourahma, Christer Aakeroy, Colin Groom, Joel Bernstein.

Below, l to r: Prashant Chopade, Ray Davis, Larry Falvello, Gary Enright, Wonyoung Choe, Daniel Adsmond, Louise Dawe, Nicholas Deifil, Onome Ugono, Janeth Presores, Claire Cook, Moqing Hu.

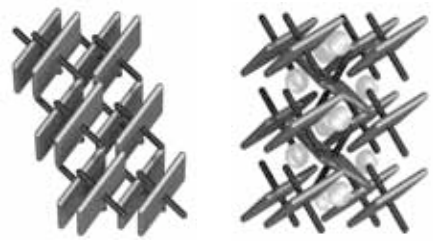


6.01 Supramolecular Chemistry, cont'd

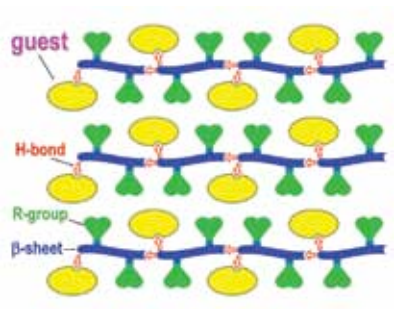
James Wuest, U. Montreal, told about engineering non-covalent motifs within purely organic solids; primarily host-guest chemistry. With simple design principles and seeming ease the Wuest group achieved their supramolecular targets despite the fact that the covalent synthesis of the individual molecules was far from trivial. **Joel Bernstein**, Ben-Gurion U. of the Negev, discussed polymorphism. Co-crystallization reactions are an effective way of generating new polymorphs. For example, a seemingly straightforward supramolcular assembly process failed, but generated numerous polymorphs or solvates of one of the two reactants. Valuable information about the role that additives play in promoting/preventing the appearance of specific crystal forms was thereby gained.

Menahem Kaftory, Technion U., and **Dejan-Kresimir Bucar**, U. Iowa, both discussed solid-state based photochemistry; the two talks complemented each other very well and also illustrated the versatility of using the organic solid state as product-controlling medium for photo-induced synthesis.

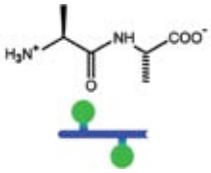
Dmitriy Soldatov, U. Guelph, and **Alicia Beatty**, U. Missouri, St. Louis, are both interested in applications based upon porous materials and their talks showed how very different building blocks can produce materials with useful and accessible space. The connection between molecular structure and physical properties is especially important in the pharmaceutical industry. The images below are from Dmitriy Soldatov.



Van der Waals packing of molecules in the crystals of guest-free [Ni(DBM)$_2$Py$_2$] complex (left) and [Ni(DBM)$_2$Py$_2$]*2(acetone) inclusion compound (right). The molecule of the complex is schematically represented by a rectangular platform penetrated by a rod and the molecule of acetone by a grey ball



The formation of inclusion compounds by hydrophobic dipeptides: guest molecules are incorporated in the interlayer space between H-bonded peptide ß-sheets



Safiyyah Forbes, Kansas State U., and Heba Abourahma, College of New Jersey, described how co-crystals of pharmaceutically active ingredients (API's) represent new solid forms that may offer real solutions to many intractable problems regarding solubility and stability of API's. According to Colin Groom, CCDC, the Cambridge Structural Database continues to expand, not only in the number of structures contained, but also with respect to new software. Their tools for translating extensive structural data into useful information are practical, easy to read and transferable. Finally, **Christer Aakeröy**, Kansas State U., managed to provide a straight answer to the title of his own presentation: *Are there really any reliable and versatile strategies for co-crystal synthesis out there?*

Christer Aakeröy and Gary Enright

6:02 & 6:15: Energy Related Materials

Session 6.02, l to r: Huimin Liu, Gregory Halder, Jason Hodges, Haiyan Chen, Jae-Hyuk Her.

Due to the large number of abstract submissions this half-day session was converted to two half days sessions; both covered work on materials related to hydrogen storage, battery and fuel cell related materials. **Session 6.02** was comprised of all contributed talks. **Jason Hodges**,ORNL,proposed a new mechanism for hydrogen absorption and desorption in lithium imide/amide systems. The next two talks by **Jae-Hyuk Her**, NIST & U. Maryland, and **Antonio dos Santos**, ORNL, covered the intricacies of various crystal structures of borohydride compounds. We also heard about *in-situ* characterization of thermoelectric and framework materials from **Haiyan Chen**, NJ Inst. Tech., and **Greg Halder,** Argonne.

Session 6.15, l to r: Ashfia Huq, Steve McIntosh, Gerbrand Ceder, Peter Feng.

In **Session, 6.15**, **Steven McIntosh**, U. of Virginia, presented an extremely convincing argument for studying fuel cell materials by means of *in-situ* scattering techniques to elucidate the mechanism of ion transport in various electrodes and electrolyte materials. There has been a long-standing interest in being able to predict crystal structures to develop new materials. **Gerbrand Ceder**, MIT, reported on the efforts of his group to predict structure based on a learning algorithm. Many success stories! Gerbrand and his colleagues predict crystal structures by a combination of data mining and *ab initio* methods. Gerbrand used the application of Li-storage electrodes for rechargeable batteries to illustrate how crystal structures determine properties such as voltage, charging rate capability, and capacity fade.The powder SIG **Margaret C. Etter Student Lecturer Award** winner **Matt Beekman**, U. South Florida, presented his work on intermetallic clathrates using x-ray powder diffraction.

Ashfia Huq

L to r: Bretna Hackert, Marvin Hackert, Sine Larsen, Louis Delbaere, Carol Delbaere. Photo by Peter Müller.

L to r: Wah Chiu, Matthew Baker, Cezar Khursigara, Dmitri Svergun, Laurie Betts, Mark Hunter, Dina Schneidman, Hiro Tsuruta.

6.03 Complementary Methods for Macromolecular Crystallography

Dmitri Svergun, EMBL-Hamburg, gave a review talk on physical principles of solution x-ray/neutron scattering including recently developed computational techniques to interpret solution scattering data. He gave several examples in which low resolution techniques complemented crystallographic studies, especially when studying flexible structures and protein complexes. He concluded with their on-going high-throughput solution scattering studies.

Dina Schneidman, UCSF, highlighted a new computational approach to study protein-protein interactions based on small angle x-ray scattering and/or cryoelectron microscopy (cryoEM). Atomic-resolution structures with electrostatic potentials from, for instance, homology modeling, are used to assemble a protein complex to fit the experimental data. The method incorporates other types of data, such as cryo-EM 2D images or 3D maps, binding site residues, and distance restraints, and is utilized in their integrated modeling program (IMP).

Mark Hunter, Arizona St. U., presented an impressive nanocrystal powder diffraction study of Photosystem I. A micro-jet device sent nanocrystals, each containing only several thousand unit cells, into a soft x-ray beam while power diffraction patterns were recorded. This study demonstrates that fewer unit cells than have previously been used in micro-beam diffraction studies can give sufficiently strong diffraction to enable structural analysis. Single crystal diffraction experiments using a hard x-ray free-electron laser beam are planned later this year.

Matthew Baker, Baylor, spoke about an effective approach to obtain near-atomic resolution structures by cryoEM. He presented a computational method, now incorporated into the program suite Gorgon, that enables visualization of secondary structure elements in electron density maps. In a recent chaperonin study Gorgon successfully displayed more than 70% of the amino acid side chains

Cezar Khursigara, U. of Guelph, reported the spatial distribution and molecular architecture of the *C. crescentus* chemoreceptors *in situ* by cryo-electron tomography. Docking of the atomic resolution trimer model for *E. coli* into the *C. crescentus* electron density map revealed the chemoreceptors organized as trimers of receptor dimers in hexagonally packed arrays within the cytoplasmic membrane. He proposed that the order/disorder of the hexagonal assembly plays a key role in dynamic activation and adaptation steps of bacterial chemotaxis.

Laurie Betts, U. of Pittsburgh, presented an excellent example of how the combination of cryoEM, and either NMR or x-ray crystallography can reveal the properties of complex virus assemblies. Docking of high resolution structures into an EM density map demonstrated how different conformations of the flexible capsid protein create different interfaces between parts of the protein. This determines how the symmetrical rings interact long-range to form different types of large assemblies. Laurie also described an EM study on microscopic crystals of a viral capsid protein that helped to explain the role of capsid interactions in the crystallization process.

Hiro Tsuruta & Wah Chiu

Index of Advertisers

L to r: Alex Ghetu, Eddy Arnold, Peter Colman, Joseph Bauman, Pamela Williams, Duncan McRee, Cele Abad-Zapatero, Brian Mark.

6.05: Structure Based Drug Deisgn

This year Fragment-Based Screening (FBS) as applied to drug discovery was emphasized. **Duncan McRee**, Sorrento Technologies, gave a short introduction to the method and introduced several key concepts.

Joe Bauman, Rutgers, discussed some exciting results of FBS on HIV-1 reverse transcriptase. The power of FBS to find novel binding sites was clearly demonstrated, as several of the sites he found had been induced by the fragment. (The site was not evident in the unbound form.) Hopefully these results will lead to some novel leads against HIV.

Pamela Williams, Astex Therapeutics, reported on several compounds which are in or near clinical trials, all produced by FBS. She discussed the methodology used by Astex to rapidly produce drug candidates.

Peter Colman, The Walter & Eliza Hall Inst., talked about antivirals and the problem of drug resistance. His talk was particularly timely considering all the recent media attention to the H1N1 pandemic. Peter discussed the characteristics of compounds that show the least likelihood of being resisted by the virus - valuable information for drug design.

Celerino Abad-Zapatero, U. Illinois, Chicago, discussed new ways of plotting and analyzing FBS data. He presented a new way of plotting ligand efficiency, i.e. the amount of binding energy per heavy atom of a ligand. Cele's method normalizes the binding of compounds according to molecular size by including the number of polar atoms in the equation. He demonstrated that these plots give valuable information on the probability that a given compound will have the proper properties for "drug-likeness".

Alexandru Ghetu, Ontario Cancer Inst., discussed finding an inhibitor of protein-protein interactions, a particularly challenging problem in drug discovery. He presented some remarkable progress in designing inhibitors against that disrupted a protein-protein interface.

Finally, **Brain Mark**, U. Manitoba, revisited the topic of resistance, this time against ß-lactam antibiotics. His approach is to shut down the induction pathway of the ß-lactamase and thus keep the antibiotics effective longer. He showed the structures of several new compounds that seem promising.

Duncan McRee and Eddy Arnold

l to r: Joseph Tanski, Carla Slebodnick, Frank Fronczek, Amy Sarjeant, Gregory Ferrence, Victor Young.

6.06: Would You Publish This?

A very entertaining evening was had as presenters "aired their dirty laundry" in an effort to stimulate discussion about how small molecule crystallographers handle problem crystal structures of chemical importance.

Cont'd, opposite page.

Would You Publish This, cont'd

Issues of disorder, solvent loss, and inherently bad data were dealt with first. **Joe Tanski**, Vassar College, had a very appropriate quote from A. L. Spek …*it looks like there exists some kind of conservation law for the sum of 'interesting structure' and 'quality structure'*… Joe continued by presenting the structure of a mixed-metal [ruthenium(III)-platinum(II)] trimer that, after substantial crystal screening and handling the data with twinning software and Squeeze gave a 'bad' structure model by IUCr standards, but a very useful structure to the eyes of the chemist.

Carla Slebodnick, Virginia Tech, presented the structure of a series of cryptand based host:guest complexes that typically have disordered cryptand, solvent, and counter anions giving inherently bad data. Use of Squeeze and various software restraints helped with the structure models, but in the end, there is no substitute for good data.

Frank Fronczek, Lousianna State U., presented *Barely Publishable (?) Porphyrin Structures*. In fact these structures were barely solvable and good refinements were not possible. Yet, the poor crystallographic results provided crucial information to chemists. **Amy Sarjeant**, Northwestern U., presented a MOF (Metal-Organic Framework) structure that required substantial fiddling with restraint and Squeeze to handle disordered linker groups and disordered solvent in the MOF cavities.

Gary Enright, NRCC, summarized the challenges in obtaining the structure of a poorly diffracting bioactive natural product derivative.

Pseudo-symmetry issues followed. **Greg Ferrence**, Illinois State U., presented "quasiracemate" structures where 2 compositionally different pure enantiomers of opposite chiral sense but similar structure cocrystallized in a 1:1 ratio with pseudo-inversion symmetry. **Victor Young**, U. Minnesota, presented several crystal structures of enantiopure substances with pseudo-inversion symmetry. Some refined well in the corresponding acentric space group while other refinements were decidedly unsatisfactory.

Subsequent discussion topics included: (a) the effort required to generate incremental improvements in structure quality, (b) methods to ensure the experimental details are included in the publication by the chemist, and (c) Squeeze (when is the program appropriate and does it bias the structure model?). In summary (and paraphrasing Frank Fronczek), - simple rules for success include not overanalyzing the data, being straightforward and honest when presenting results, and stressing to reviewers that better results are not possible.

Please join us for further discussion in the Would You Publish This II? session at the Chicago ACA meeting in 2010!

Carla Slebodnick

L to r: Eiji Takayama-Muromachi, Jasmine Millican, Dirk Johrendt, Simon Kimber, Taner Yildirim, Kenneth Littrell, John Mitchell.

6.07: Superconducting Materials:

Superconductivity is a multidisiplinary branch of condensed matter science involving crystallographers, chemists, physicists and materials scientists.

The rapidly evolving field of Fe-based superconductivity has, in the 18 months since the JACS publication by Hideo Hosono on $LaFeAsO_{1-x}F_x$, resulted in more than 1000 papers. Accordingly, Fe superconductors were the main focus of the session. **Dirk Johrendt**, Ludwig Maximilans U., described the four main families of Fe-based superconductors, identifying the links between crystal structure and the maximum transition temperature, Tc; apparently making the $FeAs_4$ tetrahedra as regular as possible is critical for obtaining the highest Tc. Johrendt used reciprocal space to argue that Fermi surface nesting effects in the $BaFe_2As_2$ family - which favor a competing spin density wave ground state - become less pronounced upon doping with K, one way to induce superconductivity. He reported that attempts to apply cuprate superconductor lessons by making compounds with higher anisotropy have yet to yield new Fe-based superconductors. He left the audience with an open question: is the essential parameter for inducing superconductivity in the Fe-based systems charge doping or structure modification?

Simon Kimber, Helmholtz-Zentrum Berlin, described neutron scattering studies on the $BaFe_2As_2$ system under pressure, demonstrating that the Fe-As bond is quite incompressible. This behavior contrasts with the high-Tc cuprates and implies that little charge transfer occurs between the Fe and As sites either as a function of doping or pressure. He also showed that the lattice constants under pressure scale with those from K-doping, which answered Johrendt's question. Apparently structure rather than the charge doping is the critical parameter for superconductivity.

On the theoretical side, **Taner Yildirim**, NIST, argued that conventional phonon-driven superconductivity is extremely unlikely in the pnictides. However, his calculations show that a close coupling between the magnetic moment on Fe and the bonding between As pairs along the c-axis could imply magnetically-enhanced phonon coupling. His calculations also provide a natural explanation for the appearance of a high pressure 'collapsed' tetragonal phase that is non-magnetic: pressure effectively 'squeezes out' the magnetism by enhancing the As-As hybridization.

John Mitchell

L to r: Victor Young, Christine Beavers, Richard Staples, Christian Graf, Vaclav Petricek, Charles Campana, David Rae.

6.08: Problem Structures: Solution and Refinement of Difficult Small Molecule Structures

Christine Beavers, Advanced Light Source, LBNL, discussed the benefits of using the synchrotron when twinned and/or highly disordered crystals result in poor diffraction at home. Problematic crystals perform significantly better using the high flux of the synchrotron, but solving many of the fullerene type structures studied nevertheless required ever-so-painful modeling. **Christian Graf**, U. Waterloo, spoke about the trials and problems associated with incommensurately modulated structures. **David Rae**, Austrailian Nat'l U., discussed the effects that layer stacking can have on space group and unit cell determination in *For a Commensurately Modulated Structure, Different Index Conditions can see Different Average Structures*.

Partha Das, U. Zurich, was awarded the Service Crystallography SIG Student Lecturer Award, Partha, and his coworkers studied the diffraction of the unstable, apparently cubic, α-phase form of $NaLuF_4$ using synchrotron radiation. (The low temperature β-form is stable and crystallizes in a hexagonal space group.) They deduced that the highest possible symmetry is tetragonal, and 6-fold twinning accounts for the apparent cubic symmetry.

6.09: Refinement Software; Difficult Refinements

The session began with **Garib Mushudov** , U. of York, describing the newest improvements to REFMAC with special attention to the treatment of automated NCS restraints and automated treatment of twinning. Paul Adams, LBL, U. California, Berkeley, focused on refinement in PHENIX and new operations including a dramatically improved new GUI.

Gerard Bricogne, Global Phasing Ltd., described a major improvement to autoBUSTER; one of the session organizers downloaded autoBUSTER and tried it while in Toronto. He was happy to report that the new version generated better statistics and a better map than had been previously obtained (not using BUSTER/TNT).

Axel Brunger, Stanford U., and coworkers developed a general geometry-based algorithm that uses a deformable elastic network (DEN) to restrain sampling to prior knowledge of an approximate or homolgous structure. DEN much improved their refinements.

Those who missed the JANA workshop were treated to a great lecture by **Vaclav Petříček**, who gave a useful explanation, using a real sample, of super space groups, and a recent solution algorithm: charge flipping. **Victor Young**, U. Minnesota, introduced us to the effects and realities of crystal structures that have a high Z' value. He explored the possible pseudo-symmetry in some of these structures and showed us the various types that could be imposed. **Chuck Campana**, Bruker-AXS, discussed approaches similar to molecular replacement that can be used to solve small molecule crystal structures. Taking advantage of the FRAG command in the SHELXL software to search with a known fragment of a compound resulted in phasing sufficient to retrieve the rest of the structure.

Richard Staples

All photographs on this page were taken by the ACA staff photographer, Peter Müller.

Session Chair Ed Collins, at right.

Dusan Turk, Jozef Stefan Inst., Slovenia, described real space refinement and automated non-crystallographic symmetry (NCS) in MAIN with a focus on the importance of accurately describing the NCS operators. **Oliver Smart**, Global Phasing Ltd., reported that local structure similarity restraints (LSSR) allows one to use known structures to better describe a set of restraints for new structures. **Edwin Pozharski**, U. Maryland, described how model ensembles could be used to determine precision in the structures that are determined using SHAKERR.

P. Horanyi would like to acknowledge and thank the ACA and Rigaku for assistance in travel funds for this meeting.

Ed Collins and Peter Horanyi

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L to r: Craig Ogata, Michel Fodje, Sebastian Boutet, Ronald Ruth, Clemens Schulze-Briese, Li Yang, Marc Allaire.

6.10 Instrumentation: Sources, Optics, Robotics and Detectors

Ronald Ruth, Lyncean Technologies Inc., talked about the Compact Light Source (CLS), a miniature synchrotron using inverse Compton scattering to produce x-rays. The cover of *Journal of Synchrotron Radiation* (Jan.2009) showed several images obtained with differential phase contrast and dark field contrast as well as the usual absorption contrast. The first structure using data collected with the CLS has been deposited in the PDB (3IFT). The CLS prototype is now shut down and the Lyncean team is installing Beta CLS, which will be up and running in a few months.

Sebastien Boutet, SLAC, reported on the status of LCLS, the new linac coherent light source at SLAC which is the world's first hard x-ray free-electron laser beam. The LCLS will be available to users based on the scientific merit of their proposals; the extreme peak brilliance will greatly enhance temporal and spatial resolution; and the expectation is that nanometer-sized crystals could be used.

Clemens Schulze-Briese, Swiss Light Source (SLS), reported on protein crystallography beamlines X06SA, X10SA and X06DA. In particular, X06SA features PILATUS 6M, the first large area pixel detector. It combines the data accuracy of counting detectors with very high count rates. In addition it exhibits an excellent point-spread-function and supports frame rates of up to 12.5 Hz, allowing for continuous shutter-free data acquisition and fine-phi slicing. The beamlines are equipped with CATS robots for automatic sample changing and in-situ diffraction screening of crystallization plates.

Michel Fodje, Canadian Light Source. The Canadian Macromolecular Crystallography Facility (CMCF) serves more than 60 protein crystallographers. Beamline 08ID is efficient and flexible, and satisfies the requirements of most protein experiments, i.e. small crystals with large unit cell dimensions. Beamline 08B1 is a bending-magnet beamline for high-throughput crystallography. Michel reported the first diffraction images collected on 08B1. Stanford-type automatic sample changers enable high-throughput and remote data collection.

Lin Yang, Brookhaven, presented data collected during commissoning of the X9 beamline at the National Synchrotron Light Source. X9 is microbeam capable (<10 microns). The energy range is 2.1 to 20 KeV. Two sets of K-B focusing mirrors are utilized to give the users the flexibility of choosing between small beam divergence and small beam spot size at the sample. Both small and wide angle data can be collected simultaneously. A hexapod is used for positioning during sample rotations.

Wayne Hendrickson, Columbia U, reported on the new synchrotron source under construction at Brookhaven: the National Synchrotron Light Source II (NSLS-II). which will be capable of x-ray beams of 1 nm size and 0.1 meV resolution. The exceptional brightness and high capacity of NSLS-II will provide unique opportunities in life sciences. Plans for diverse biological applications, including x-ray crystallography, x-ray scattering, imaging and spectroscopy are being formulated.

Jesse Smith, U. of Ottawa, received the synchrotron SIG **Etter Student Lecturer Award**. Jesse described two experimental techniques in exploiting area detectors to reduce Compton scattering via energy selection and to measure beamline polarization. The first takes advantage of the abrupt discontinuity in absorption as a function of energy due to barium, the primary compositional element of the imaging plate phosphor. Using a selected energy, 35% improvement in signal-to-noise ratio is observed. The second technique to measure beamline polarization, takes advantage of the scattering dependence as a function of the detector azimuthal angle.

Marc Allaire, at right, presenting the Synchrotron SIG Etter Student Lecturer Award to Jesse Smith

Gabriella Carini, Brookhaven, spoke about the new generation of x-ray active matrix pixel sensors (XAMPS) which has been developed at BNL. The XAMPS is a position sensitive ionization detector-made on high resistivity silicon. It consists of a pixel array detector with integrated switches. Prototypes of 64 x 64 pixels have been tested and are reaching the specs of low noise and dynamic range required. A final detector of 1024 x 1024 pixels will be part of the x-ray pump probe instrument at the LCLS at SLAC.

Jean-Luc Ferrer, Institut de Biologie Structurale, reported on the G-Rob system developed on beamline FIP-BM30A at the ESRF. G-Rob is a continuation of the CATS system (Jacquamet et al, JSR 16 (2009), 14-21), a sample changer currently being installed at multiple synchrotrons. G-Rob utilizes a 6-axis robotic arm to perform transfers and data collections on frozen samples and can also do screening.

L to r: Craig Ogata, Gabriella Carini, Ruslan Sanishvili, Jesse Smith, Christian Rieckel, Jean-Luc Ferrer, Timothy Graber, Wayne Hendrickson, Marc Allaire.

Christian Riekel, European Synchrotron Radiation Facility, a pioneer in microdiffraction at the one and sub-micron scale, reported on beamline ID13 at the ESRF. Pushing the limits to smaller biological objects and smaller beam sizes requires the integration of novel sample environments. Christian described diffraction from micron-sized crystals and microSAXS experiments using microfluidics technology. He touched on the many optical techniques and innovative instruments that now propel micro-diffraction towards the nano-scale, a development that will require exhaustive experimental studies as well as continued collaborations between scientists in the field

Ruslan Sanishvili, Argonne, designed experiments to check if a 1μm x-ray beam would reduce the radiation damage to macromolecular crystals during data collections. A one micron beam was achieved at the GM/CA-CAT facility by removing the beam focusing mirrors and inserting a Fresnel zone plate as a focusing element at ~15 keV energy. However, no significant decrease of damage was observed in lyzozyme crystals. In accordance with theory, the damage was greater along the polarization vector than in perpendicular direction and did not extend beyond 4 μm from the incident beam center.

Timothy Graber, U. of Chicago, presented an overview of the BioCARS beamline at the Advanced Photon Source. Recently upgraded, the facility has been optimized for pump-probe time-resolved x-ray diffraction. For these measurements, a 100 picosecond x-ray pulse containing ~1010 photons is isolated and focused to a 90mm (H) by 20mm (V) spot size. Additionally, a new picosecond laser system and storage-ring synchronization scheme has been commissioned. Tim described a time-resolved experiment with dimeric *Scapharca Inaequivalvis* (clam) hemoglobin that utilized both crystallographic and WAXS techniques and showed how complementary information can be extracted to provide a better understanding of the photocycle for this system.

Marc Allaire & Craig Ogata

lL to r: John Mitchell, Andrei Savici, Despina Louca, Graham King, Gregory Halder, Pierre Bordet, Bruce Gaulin, Ovidiu Garlea.

6.11: Cooperative phenomena in magnetic materials

Recent research has used neutron or x-ray scattering to probe the structure and magnetic phase diagrams of a variety of strongly correlated electron systems. **Bruce Gaulin**, McMaster University, opened the session with a presentation of two magnetic pyrochlore oxide materials, $Er_2Ti_2O_7$ and $Yb_2Ti_2O_7$, which can be thought of as XY-like moments decorating a network of corner sharing tetrahedra. In both materials the geometrical frustration is expected to lead to strongly fluctuating phases without static order. In spite of their structural similarities, their behavior in magnetic field is strikingly different: while in $Yb_2Ti_2O_7$ the disordered ground state can be brought to order, the long range ordered magnetic state in $Er_2Ti_2O_7$ can be destroyed by application of modest magnetic fields.

Pierre Bordet, CNRS Grenoble, France, continued with another very intriguing class of materials: the Fe based langasites of type $A_3BFe_3D_2O_{14}$ with A=Ba, Sr, Ca; B=Ta, Nb, Sb and D = Ge, Si. These are structurally chiral compounds in which the Fe cations form planar triangular lattices of triangle units. It was shown that their magnetic structure can be modeled by a helical spin arrangement propagating along the c axis of equal moments lying in the (a,b) plane at 120° from each other within

cont'd, next page

6.11: Cooperative phenomena in magnetic materials, cont'd

each triangle. Unpolarized neutron scattering on a single crystal associated with spherical neutron polarimetry proved that a single triangular chirality together with a single helicity was stabilized in a crystallographically enantiopure crystal.

Andrei Savici, Johns Hopkins U., made a smooth transition from frustrated magnetism to stripe models in short range charge and spin superstructures. Particular emphasis was placed on elastic neutron scattering measurements of short range spin and charge order patterns in compounds similar to {214} high-temperature superconductors. The measured diffuse magnetic scattering was compared with the predictions of several simple models of disorder competing with the long range supperlatice coherence. **Despina Louca**, U. of Virginia, discussed uncharacteristic phase separation in Cobaltites. Her systematic neutron scattering measurements on single crystals of $La_{1-x}A_xCoO_3$ ($A = Ca^{2+}$, Sr^{2+} and Ba^{2+}) revealed the development of magnetic superstructures, which are strongly dependent on the size of the A-site dopant in an unusual way. The tendency towards coexistence of competing ferromagnetic and antiferromagnetic orders increases upon increasing the radius of the dopant, giving rise to an inhomogeneous ground state.

John Mitchell, Argonne National Laboratory, gave an engaging talk about the preparation and properties of a new multiferroic material, namely, the high-pressure phase of $FeTiO_3$. His quest for this new phase has been stimulated by recent density functional theory calculations, which predicted that the family of compounds $MTiO_3$ (M = Mn, Fe, Ni) are promising candidates where a polar lattice distortion can induce weak ferromagnetism. **Graham King**, Ohio State U., followed with a presentation on the magnetic structures of three NaLn $MnWO_6$ (Ln=La, Nd, Tb) perovskites, determined using neutron powder diffraction. Each of these compounds possesses a rock salt ordering of the Mn^{2+} and W^{6+} ions and a layered arrangement of the Na^+ and La^{3+} ions. He showed that an incommensurate magnetic ordering occurs when Ln is magnetic and discussed the interplay between the Mn^{2+} and Ln^{3+} magnetic sublattices.

Gregory Halder, Argonne National Laboratory, reported on a magneto-structural investigation of the molecular -based antiferromagnet $CuF_2(H_2O)_2$(pyrazine) using synchrotron-based powder diffraction and magnetic susceptibility measurements at high pressures. His studies have revealed a remarkable sequential reorientation of the Jahn-Teller axis, and consequently the magnetic coupling interactions, as a function of pressure.

Ovidiu Garlea

6.12 Professional Directions

Is there a future for crystallography? A panel of six crystallographers employed in academics, government, and industry answered this question with a resounding "YES!"

The members of the panel answered questions regarding the many professional avenues available to budding crystallographers. The panelists were: **Steve Ginell**, SBC-CAT @Argonne Labs, **Jim Kaduk**, INEOS Technologies, **Steven Sheriff**, Bristol Myers-Squibb, **Charlotte Stern**, Northwestern U., **Paul Swepston**, Rigaku Americas, **Carrie Wilmot**, U. of Minnesota, and **Mark Wilson**, U. of Nebraska-Lincoln. Around 100 people attended the session. A large majority of attendees were young scientists and first timers to the ACA meeting. Many of the questions asked addressed concerns connected to the tumultuous economy and career options in crystallography. The panelists were very optimistic about future opportunities and shared many personal stories to illustrate how they were able to succeed in their careers.

The panel counseled that the best way to find success in a scientific career is to pursue that which you are most passionate about. It was recognized as well that interests and strengths transform over time and a willingness to accept change allows great opportunities to arise. One of the most common themes found among the personal stories of the panelists was that each had a mentor that was there for them to give advice and support at career crossroads. This theme accentuated the importance of seeking out collaborations and involvement in the scientific community in order to build relationships.

This was a very wonderful session where many ideas and advice were exchanged. There was a very positive feeling after the panelists concluded and many attendees stayed after to ask more direct questions of panelists. We are excited that a similar session, "Professional Odysseys", aimed at informing young scientists of career options and advancement opportunities will be held next year at the 2010 Chicago meeting.

Ryan Jackson and Herb Klei

L to r: Svilen Bobev, Marilyn Olmstead, Bruce Noll, George Sheldrick. Photo by Peter Müller.

From left: Michael Engel, George Sheldrick, Carol Brock, Patrick Loll, Anna Gardberg, John Warren, Marilyn Olmstead, Ilia Guzei, Peter Stephens, Christine Beavers. Photo taken using Ilia Guzei's camera.

6.13: Large Small Molecules

George Sheldrick, Georg-August-Universität, Göttingen, opened by discussing the performance of his dual space approach with the more recent charge flipping methods. In the dual space approach, (when heavier atoms are present, the Patterson function is used to obtain plausible starting coordinates), dual space recycling is followed by cycles expanding to the full data. George emphasized that charge flipping uses all the data but that it is critical to have a high resolution dataset.

Marilyn Olmstead, UC Davis, reported on the refinements of disordered fullerene structures using FRAG/FEND and AFIX commands of the SHELXL package. Her largest cage fullerene (104 atoms) with two samarium atoms within the cage is a striking example. **Patrick Loll**, Drexel U., described the successful phasing of a large molecule (2550 Da) with one chlorine atom when a ferrocene derivative was used to facilitate the process. He also emphasized the importance of high resolution (1.4 Å) data.

Anna Gardberg, ORNL, spoke about using both deuterated and non-deuterated crystals of rubredoxin to locate H atom positions via combined neutron and x-ray diffraction data. The utilization of neutron data resulted in an eightfold improvement in the visualization of H atoms; however the use of very high resolution data (~0.75 Å) may not be advantageous. Anna posed a question: *At what resolution do you lose the advantage of using neutrons?*

Carol Brock, U. Kentucky, discussed commensurately and incommensurately modulated structures with Z' (read "zed") > 1; she suggested reasons (such as important conflicts between packing tendencies) as to why and when modulation occurs. Carol pointed out that it is advisable to consider incommensurate modulation when $Z' \geq 5$.

Michael Engel, Diamond Light Source, UK, described the small and macromolecular experimental setup at the Diamond synchrotron source concentrating on instrument configuration, functionality, 80-sample robots, and diffractometer parameters. **John Warren**, U. Bath, UK, described possible experiments with an environmental gas-cell for studies of "Chinese lantern" - type complexes of Fe/Co/Ni that can accumulate, retain, and release SO_2. John showed the gas-cell design and examples of controlled variables that can influence the experiment.

Peter Stephens, SUNY-Stony Brook, demonstrated how, lacking single-crystal data, structures of small proteins can be solved by powder diffraction when simulated annealing and model building are expertly executed.

Christine Beavers and Ilia Guzei

Above: Hakon Hope at right talking with Bruce Noll. Below: Victon Young taking photos. Photos by Peter Muller.

Ilana Goldberg and Onoma Ugono at opening reception

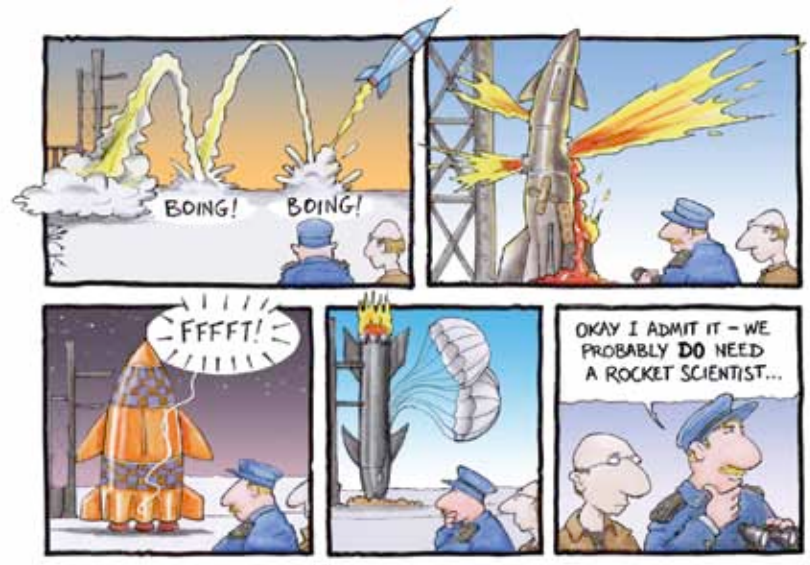
L to r: Xiaoping Wang, Christina Hoffmann, Brian Toby, George Sheldrick, Regine Herbst-Irmer, Joe Reibenspies, Vaclav Petricek.

6.16: Tips & Tricks of the Computing Trade

George Sheldrick, U. Göttingen, gave a detailed description of the algorithm used in the CELL_NOW program for indexing twinned crystals. He also discussed the computational aspects of solution and refinement of problem structures, in particular of twinned crystals, using open source SHELX and Bruker-AXS SHELXTL. **Christina Hoffmann**, ORNL, demonstrated new visualization tools now available in the ISAW (Integrated Spectrum Analysis Workbench) software package for time-of-flight Laue single-crystal neutron diffraction. ISAW has been developed for the new generation time-of-flight single crystal neutron diffractometers (SCNDs) at the spallation and steady state sources at ORNL.The new SNCDs are capable of measuring x-ray size samples with high sensitivity to hydrogen atoms and magnetic scattering. **Vaclav Petricek**, Inst. of Physics, Academy of Sciences of the Czech Republic, presented examples using JANA2006 to analyze the long range order (modulation) as well as the atomic disorder (non-harmonicity/ anharmonicity) in crystal structures.

Joseph Reibenspies, Texas A & M, showed some tricks for writing simple GUIs for legacy crystallographic programs that should help crystallographers to stay close to the problem they want to solve. **Regine Herbst-Irmer**, U. Göttingen, reported her high resolution structure of 9-diphenylthiophosphinoyl-anthracene. The conventional aspherical atom approach leaves ghost peaks around heavy S atoms; these residual peaks disappeared only when Gram-Charlier anharmonic coefficients were introduced. Finally, **Brian H. Toby**, APS, ANL, gave an update on software development efforts in the GSAS program suite. The proposed new GSAS-II program package will be built with an open framework and will be extensible. Once developed, the program will be easy to use and will benefit the powder diffraction community.

Xiaoping Wang



Cartoon courtesy of Nick D. Kim, who is an analytical environmental chemist who currently works for Waikato Regional Council. He is an honorary lecturer at the University of Waikato in New Zealand

Stephanie Pfaffen and Anson Chan at the Mentor-Mentee dinner.

L to r: Pamela Whitfield, Oladipo Omotoso, Brian Toby, James Cline, Lutz Bruegemann, Patrick Mercier.

6.17: Accuracy and Standards in Powder Diffraction

Jim Cline, NIST, who has certified all of the modern standards for powder diffraction, gave an overview of their various standards, the requirements for materials and the certification procedure to produce final standards. For more recent standards 640d and 676b, Jim had additional details on the production and characterization techniques involved, including the 'NIST traceable hammer' used to break up the single crystal silicon boules before grinding!

Lutz Brügeman, Bruker-AXS, discussed the requirements for obtaining highly accurate XRPD data. Goniometer components, geometries, optics and detectors were all considered in assessing the reproducibility that should be expected from a modern diffractometer. The correct configuration to suit the particular problem affects accuracy positively.

The quantitative analysis of clay-containing minerals using x-ray diffraction, definitely a 'black-art,' was the topic of the talk by **Oladipo Omotoso**, NRC. Difficulties and possible strategies for overcoming them were reported; for example an alternative method to spray drying that produced samples with non-orientating, spherical (and therefore easily packed) particles.

Since home laboratory data is often just not good enough, **Brian Toby**, Argonne, presented the specifications and capabilities of the 11-BM beamline at the APS. This beamline, on which excellent high resolution data for several configurations may be obtained, can be accessed through a rapid-access mail-in service. Typical data from 11-BM was presented along with an example of the on-line application for beamtime and the subsequent steps required before data is delivered to your email inbox.

Patrick Mercier, NRC, described a method for gauging the reliability of a Rietveld refinement using singular value decomposition. In conjunction with a geometrical parameterization approach to structure refinements he showed how it is possible to improve the accuracy and precision of measurements close to those obtained using single-crystal techniques.

Pamela Whitfield

At the Mentor-Mentee dinner, l to r: Sulochana Devi Baskaran, Ardian Wibowo, Leo Koharudin, Laurie Betts, Matt Hildebrandt.

L to r: Seung-Hun Lee, Chris Stock, Sungdae Ji, Peter Gehring, Jinsheng Wen, Valery Kiryukhin.

6.18: Ferroic & Multiferroic Materials

Ferroic materials include ferroelectrics, ferromagnets, and ferroelastics, whereas multiferroic materials are those in which two or more ferroic order parameters are present in a single phase; as such these materials possess enormous potential for industrial device applications and have generated intense scientific interest over the past several years.

Valery Kiryukhin, Rutgers, presented the discovery (with colleagues) of a diode effect in single crystals of the multiferroic material $BiFeO_3$ in which the electric current is highly non-linear, strongly temperature dependent, and unidirectional, flowing in the same direction as the electric polarization (Choi *et al*., *Science* **324**, 63 (2009)). The diode effect can be reversed by simply switching the direction of the electric polarization with an electric field pulse. In addition, Valery showed polarized neutron scattering data that demonstrated that one could switch reversibly between one of two unique electric polarization directions, as well as the populations of equivalent spiral magnetic domains, via application of an applied electric field, a feat that has yet to be achieved in $BiFeO_3$ thin films. These results are expected to advance research on $BiFeO_3$ multifunctional devices significantly.

Multiferroicity has different origins; the multiferroicity in $BiFeO_3$ arises from the lone pair of 6s electrons on the Bi-site, which drives the ionic displacements required for ferroelectricity, and from the partially filled d-shell on the Fe-site, which contributes to the magnetism. In contrast, multiferroic behavior in $LuFe_2O_4$ stems from a charge ordering of the Fe^{2+} and Fe^{3+} ions that forms a polar arrangement in the presence of magnetic ions around 340 K. Although the ferroelectric polarization P appears above the magnetic ordering temperature, a significant change in P is observed within the magnetic phase, and this indicates the presence of a large coupling between the ferroelectricity and magnetic order. **Jinsheng Wen**, Brookhaven, the **Margaret C. Etter Student Lecturer** award winner (Materials Science SIG), discussed the extremely unusual finding that an external magnetic field can affect the magnitude and correlation lengths associated with the charge order in $LuFe_2O_4$, even at temperatures greater than the ferrimagnetic ordering temperature of 240 K (Wen et al., *Phys. Rev. B* **80**, 020403, 2009). This result provides a natural explanation for the unprecedented giant magnetoelectric response at room temperature and suggests that a different magnetoelectric coupling mechanism must be operative in this important charge-ordered multiferroic, which, given its properties, is nearly ideal for device applications.

Chris Stock, Rutherford Appleton Labs, ISIS, spoke about the relaxor compound $Pb(Mg_{1/3}Nb_{2/3})O_3$ (PMN), one of the most highly piezoelectric materials known. While PMN exhibits a ferroelectric soft mode at the zone center, it also displays short-range ordered superlattice peaks at various zone boundary locations that are consistent with antiferroelectricity and simultaneously track the temperature dependence of the ferroelectric soft mode. Using neutron inelastic scattering methods Chris and his colleagues discovered the presence of soft, highly-damped zone-boundary phonon modes located at the same reciprocal lattice positions (Swainson *et al*., *Phys. Rev. B* **79**, 224301, 2009), which indicates a dynamic origin for the superlattice peaks. Detailed structure factor calculations demonstrate that the soft zone-boundary modes are optic modes and not zone boundary tilt (acoustic) modes as might have been expected. A possible correlation between the ultrahigh piezoelectricity in PMN and the soft zone boundary modes was suggested based on a comparison with identical measurements taken on a single crystal of PMN doped with 60%$PbTiO_3$. This level of doping is sufficient to eliminate the anomalous piezoelectricity, and in this material no soft zone boundary modes were observed at any temperature.

Peter Gehring

Cartoon courtesy of Nick D. Kim, who is an analytical environmental chemist who currently works for Waikato Regional Council. He is an honorary lecturer at the University of Waikato in New Zealand

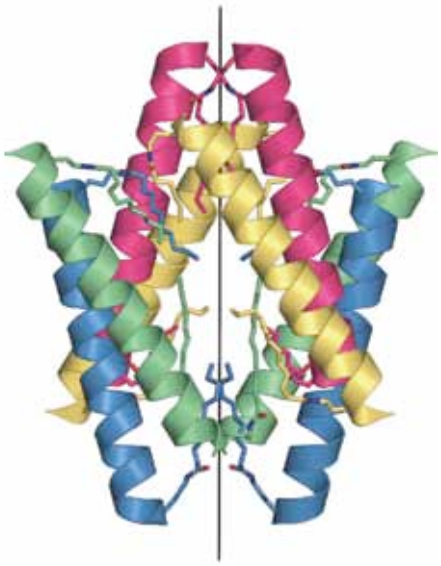
From left: David Gidalevitz, Ursula Perez-Salas, Gil Privé, Philip Kiser, Thomas Weiss.

6.19: Membranes and Associated Proteins

Topics ranged from cholesterol interactions with the lipid membrane to atomic resolution structures of membrane proteins.

David Gidalevitz, IIT, gave a detailed account of his work on the interaction of cholesterol with the DPPC monolayers. Using x-ray reflectivity he showed in near atomic resolution that at low mole fraction the cholesterol is located within the hydrophobic region of the monolayer stretching the acyl chains of the lipid. At high molar concentration the cholesterol molecules are seen to be closer to the water interface which explains the increased chemical reactivity of the cholesterol at high molar concentrations.

Ursula Perez-Salas, Argonne, presented her research on the mechanism of bicelle-based methods for membrane protein crystallization. This crystallization method uses self-assembled disc-like membranes, (bicelles), as a matrix. Ursula showed that the introduction of commonly used detergents like octylglucoside into the bicelle system significantly changes the phase behavior and structure of the system by promoting the mixing of the long- and short-chain lipids in the bicelle.



From Gil Privé: Octameric micelle of a designed lipopeptide detergent at 1.20 Å resolution, revealing most of the acyl chains in the ordered micelle interior. Crystal structure of a self-assembling lipopeptide detergent at 1.20 Å, by Ho DN, Pomroy NC, Cuesta-Seijo JA and Privé GG. PNAS 105, 12861-12866 (2008).

Gil Privé, U. Toronto, presented the functional design and high resolution crystal structure of LPD-12, a lipopeptide detergent specifically designed for the study of integral membrane proteins. This lipopeptide consists of a 25-residue peptide designed to form an α-helix with acyl chains linked to side chains located at positions 2 and 24. In solution the LDP-12 self-assembles into cylindrical micelles with acyl chains facing the inside. The chain packing in the micelle interior is designed to provide a better more stabilizing environment for membrane proteins relative to traditional detergents. The crystal structure shows that the LPD -12 forms octameric micelles in which four pairs of antiparallel LPD dimers are assembled.

Marcus Mueller, ETH Zürich, described the crystal structure of the dodecameric membrane pore formed by cytolysin A. Comparing the structure of the protomers in the pore with the structure of the monomer in solutions reveals that substantial rearrangements of parts of the monomer take place upon membrane insertion and pore formation.

Philip Kiser, Case Western, reported the crystal structure of bovine RPE65, the enzyme responsible for the *trans*-to-*cis* conversion of the retinoid during the visual cycle.

Thomas Weiss

At the Awards Banquet reception, l to r: Tony Linden, Ton Spek, Gary Newton, I.David Brown, James Golen. Photo by Peter Müller.

L to r: Mitch Luna, Felix Vajdos, Tianjun Sun, Alaji Bah, Shenping Liu, Emil Pai, Andrew Karplus.

6.20 Structural Enzymology

Andy Karplus, Oregon State U., led off with an in-depth analysis of glutathione reductase and a number of its ligand complexes at ~ 1Å resolution. Despite being the subject of investigation for more than 30 years, this enzyme still holds surprises as we probe its structure in finer and finer detail, e.g. non-planar peptide bonds and contacts very conducive for catalysis but too close for comfort (i.e. < van der Waals distances). **Shenping Liu**, Pfizer, gave an insightful presentation on phosphodiesterase 9 (PDE9). He took advantage of the less than stellar catalytic rate of the enzyme trapped intermediates in order to observe the reaction mechanism of this biologically and pharmaceutically important class of enzymes.

Alaji Bah, Washington U., the BioMac winner of a **Margaret C. Etter Student Lecturer Award**, presented a convincing synthesis of classical enzymology and structural biology in his investigation of the allosteric regulation of the serine protease thrombin. Alaji and colleagues engineered an allosteric switch into thrombin, which enhances its activity against anticoagulation substrates and ultimately helps shut off the coagulation cascade. He also stressed the importance of Na^+ ions in this process; the electron density of these ions is difficult to distinguish from that of water molecules and they are therefore often misinterpreted. **Mitch Luna**, Scripps, spoke about his work on the structural characterization of cytochrome *ba3* oxidase, an integral membrane protein. Of particular interest was his "channel-tracking" approach, which uses noble gases (Xe, Kr) as O_2 mimetics to map out the channels through which O_2 migrates from the lipophilic intramembrane region to the catalytic heme centers. He also extended the meaning of "pre-shrunk" from a purely jeans fashion-oriented term to cryoprotection of membrane protein crystals. **Tianjun Sun**, U. Calgary, using *in situ* proteolysis and a slight modification of Mary Poppins' famous line "with a little bit of lemon (citrate)", crystallized the substrate complex of a truncated version of human ATP-citrate lyase, a multi-domain protein. The resulting structure enabled him to identify the binding site and also suggest a viable catalytic mechanism. **Tim Maier**, ETH Zurich, presented a tour-de-force on eukaryotic fatty acid synthases, enormous hetero-oligomeric structures that have long eluded structural biologists due to their size and complexity. The eukaryotic version has a very different architecture from that of bacterial and *S. cerevisiae* enzymes. Tim showed a short movie that illustrated how the substrate is shuttled from one reaction center to the next.

Sine Larsen, U.Copenhagen, and IUCr President, reinforced the idea in many minds that Danish = sweet dessert, as she described her laboratory's recent work on substrate recognition and catalysis in two families of polysaccharide lyases. We not only learned which enzyme is crucial to clarify apple juice but also reaffirmed our belief that "structure does say something about function". **Kevin Kirouac**, U.Western Ontario, presented research on error-prone replication and stalling in human DNA polymerase, and described how this enzyme makes mistakes that lead to a molecular roadblock. He also "fingered" the "finger" domain as the most probable culprit in misrecognition. **Lyndal Hill**, U. Minnesota, showed how the enzyme, methylamine dehydrogenase, can, with a little help from a friend (the c-type diheme protein MauG), synthesize its own cofactor TTQ from two of its own tryptophan residues. This novel bit of biochemistry includes an Fe^{IV} Fe^{IV}oxo catalytic intermediate. **Dheeraj Khare**, U.Michigan, studied Hal, -not the chatty sci-fi computer -, but a member of the cupin superfamily and an unusual halogenase in the biosynthesis pathway of Curacin A, the major lipid component of a marine cyanobacterium and a tubulin-binding antimitotic agent. **Alberto Podjarny**, CNRS, Illkirch, combined sub-Å resolution x-ray data with neutron Laue data collected from crystals of deuterated specimens of human aldose reductase complexed with $NADP^+$ and inhibitors. He showed a fascinating view of the protonation states of active site residues. His findings agreed with a previously established MD-QM model of the proton donation mechanism. Continuing the theme, Andrey **Kovalevsky**, LANL, described how he made good use of the PCS beamline at the Lujan Center to apply time-of-flight neutron crystallography. He was able to analyze in detail exactly how xylose isomerase catalyzes the interconversion of glucose and fructose. He then proposed a revised mechanism for this enzyme, one of great importance in the food industry. **Linda Yu**, Columbia, gave a talk on *S. aureus* pyruvate carboxylase in complex with coenzyme

L to r: Linda Yu, Masahiro Fujihashi, Lyndal Hill, Felix Vajdos, Alberto Podjarny, Emil Pai, Sine Larsen, Kevin Kirouac, Andrey Kovaleysky, Dheeraj Khare.

6.20: Structural Enzymology, cont'd

A. This enzyme forms a symmetrical tetramer; CoA binding leads to a change in the BC dimer interface. She also characterized several naturally occurring mutations that lead to enzyme inactivation, and showed that some of these simply block biotin binding, while others affect catalysis. **Masahiro Fujihashi**, Kyoto U., presented "time-resolved" structures depicting the progress of a very slow (artificial) reaction catalyzed by orotidine 5'-monophosphate decarboxylase. He made an excellent case for his proposal that the enzyme's active site distorts the bond of any substituent linked to the C6 position of the substrate. He also described the covalent modification of an active site lysine by potential drug leads.

Emil Pai and Felix Vajdos

Sean Seaver, Cora Lind, Joe Trapp, Charlote Lane, Bill Duax, Jane Bednarz, Bernhard Rupp, Gary Battle, Shuchismita Dutta, Courtney McEachon, Kevin Gibas, Christine Zardecki, Jimmitti Teysir, Lorraine Malaspina, Isabel Xu, Joe Ng.

6.21: Educational Outreach in Crystallography

Eight presentations were provided to report various educational methods for effective learning and awareness in x-ray crystallography. **Christine Zardecki** and **Suchismita Dutta**, RCSB Protein Data Bank, jointly reported their outreach effort on the dissemination of structural data to students, educators and the general public. The RCSB is reaching out to secondary schools, undergraduate students and the research community using everyday-life examples showing how protein structures are associated with diseases such as hemogolobin or viruses. Immersive PDB virtual reality environment, Science Olympiad, kiosk displays, calendars and posters were among the effective tools used to excite and motivate students and the public. Content knowledge surveys, professional society meetings, demands for resources from students and teachers, and the number of repeat customers attest the effectiveness of their outreach efforts. Questions under exploration include the connection of 3D molecules to the membrane, interactions with other macromolecules and their connection to medicine. Visual art galleries, and the light show of DNA at the Olympic opening ceremony are examples of displays of 3D structures.

In the age of blog, U-tube, facebook and tweeter, **Sean Seaver**, U. Toledo, explained how the internet can provide the capability to quickly communicate ideas and provide a discussion and tutorial forum about crystallography through his blog, ***www.P212121.com***. There may be 50 ways to leave your lover but Sean highlights 10 ways to comfort a crystallographer including conquering PCR problems, expression difficulties and precipitation challenges. His blog gives crystallographers a place to discuss problems, ideas and solutions, and also explains what he has learned "the hard way" to save others from making the same mistakes.

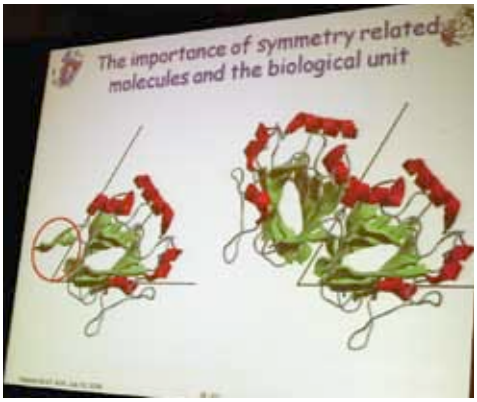
Gary Battle, CCDC, discussed outreach projects at the Cambridge Structural Database. Currently a free online teaching set of the CSD is available, and access to the CSD has been implemented in undergraduate chemistry curricula. The goal of this project is to give students an appreciation for crystallography, and make them realize that molecules are 3D objects and not flat 2D images.

cont'd on next page

6.21: Educational Outreach, cont'd

The energy and enthusiasm of young scientists was especially evident during three joint presentations by **Jimmitti Teysir**, **David Dziak**, **Dana Hogan** and **Patrick Ryan**, all Buffalo high school students mentored by **Bill Duax**. Their talks demonstrated the ability of young students to understand and perform high impact science. They discussed the possibility of a primordial genetic code that begs the question "was there a simpler code?" The ancient bacteria *Anaeromyxobacter dehalogenans* has been reported to have a simpler and more stable genetic code half the size of the universal code. This opens the possibility that it might be a billion year old living relic. An astounding conclusion was put forth stating that 3 billion years ago, a precursor to the standard genetic code used 32 codons, all ending in G or C, to encode all amino acids.

Bernhard Rupp told chilling tales from the crypt. He strongly advocated the use of real molecules to help students make the connection between crystallography, symmetry, and real life problems, instead of the common extensive abuse of meaningless objects such as ducks, piglets and horses as motifs. It is important to show the network of sparse, weak intermolecular interactions with actual structures to give learners an appreciation of the power of crystallography. Exercises using 2D diffraction gratings are a powerful tool in understanding twinning and extinction. The presentation of complex incomprehensible equations is a horror that can lead to students turning their back on crystallography. Showing visual concepts may be better for beginners. Appealing crystallographic education that will encourage students to stick with the topic and learn it properly are important if the community wants to avoid publications of hot structures in vanity journals that report models having hidden defects or are outright deceptive and wrong, leading to retractions.

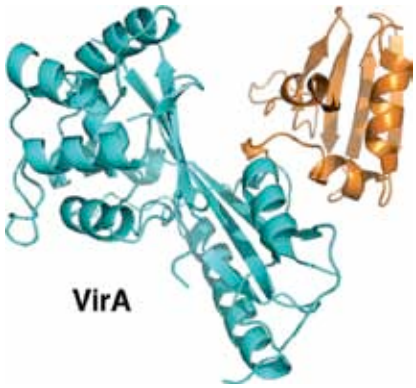


Finally, the ACA Summer School was praised by **Lorraine Malaspina,** U. Federal de Goiás, who shared her first hand experience. She made a compelling case that the school was very effective in teaching students who have limited access to formal crystallography teaching. Hands-on exercises with experienced crystallographers, and opportunities for the students to bring their own samples, collect data, and work on data analysis with one-on-one coaching by experts in the field are invaluable to all who attend. The international students especially benefit from establishing contacts with crystallographers because they can use networking to explore possible graduate studies in American universities.

Cora Lind and Joe Ng

Orphan Macromolecular Posters

There were a few dozen macromolecular crystallography posters (both structures and technique-oriented) that were not associated with any session including some up for poster prizes. These "orphan posters" reported many exciting results for a wide range of interesting systems. Here are a few highlights.



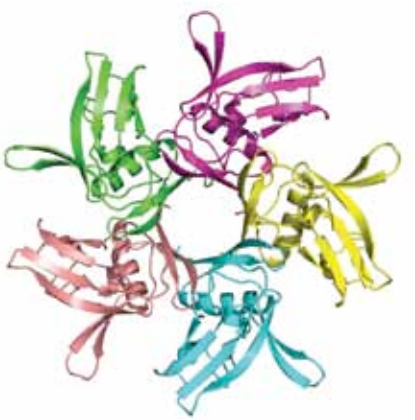
The three dimensional structure of the VirA monomer reveals two independently folded domains that resemble the letter 'V'. The partially disordered N-terminal domain is colored orange (residues 1-130), while the C-terminal domain is colored cyan (residues 131-400). The monomer consists of 12 α-helices and 12 ß-strands, including a four-stranded anti-parallel ß-sheet located in the C-terminal domain. Protein Sci. 2008 Dec; 17 (12): 2167-73.

Jamaine Davis, NCI-Frederick, showed us the structure of VirA, above, a protein involved in the type III secretion system of *Shigella flexneri* in her poster **PT001**. The structure disproved the prevailing hypothesis that VirA is a papain-like cysteine protease. The structure was described as resembling the letter "V", but this viewer, after admittedly having a few beers, thought it looked more like a heart. Anyway, more work is needed to assign the molecular function of VirA.

Joyce Wong, U. Alberta, reported the structure of TraM complexed with DNA in **PS005**.

In the prototype F plasmid, conjugation requires binding of the plasmid-encoded protein TraM to specific sites at the plasmid origin of transfer. The crystal structure of a TraM-DNA complex from the F-related plasmid pED208 reveals that two TraM tetramers bind via ribbon-helix-helix domains to its strongest binding site, sbmA. The structure provides a first glimpse into TraM-induced DNA unwinding and distortion. TraM binds cooperatively to sbmA without protein-protein contact. This cooperativity depends on the spacing between TraM GANTC binding motifs, as shown by electrophoretic mobility shift assays.

TraM is involved in horizontal gene transfer in bacteria, and it has a ribbon-helix-helix domain at the N-terminus. The structure features two ribbon-ribbon-helix dimers of the tetramer clamping DNA though the major groove.



DdrB is a protein unique to the extreme radiation resistant bacterial family deinococcus that has been shown to be essential to damage recovery. The 2.9Å structure of DdrB from Deinococcus geothermalis reveals its N-terminal oligomerization motif that coordinates its pentamer formation in solution, as well as a novel fold for ssDNA binding.

Seiji Sugiman-Marangos, McMaster U., PT018, showed an amazing pentameric ring structure of five monomers of the protein DdrB (DNA Damage Response B) from *Deinococcus geothermalis*;

This organism can quickly recover from DNA double-strand breaks induced by desiccation and exposure to ionizing radiation. A careful, manual alignment of DdrB with *E.coli* SSB revealed remarkable overlap between 4 ß-strands involved in ssDNA binding. Indeed, as shown by electrophoretic mobility shift assays, DdrB binds to single-stranded but not double-stranded DNA *in vitro*. Rather than ssDNA threading through the central pore of the pentamer, a model was presented where the ssDNA binds to the top face of the pentamer along the solvent-exposed surface of a *ß*-stranded sheet. We eagerly await a future crystal structure of DdrB with ssDNA.

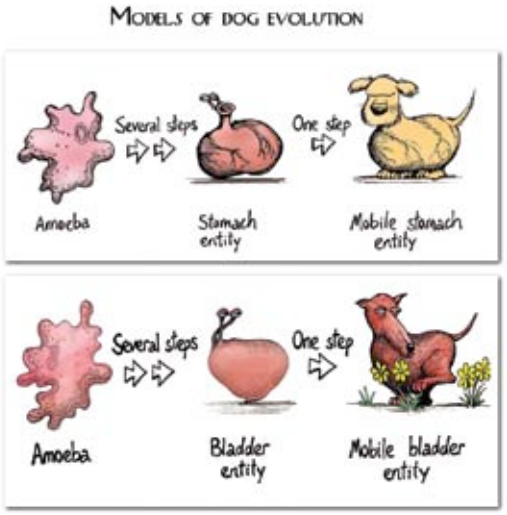
Models of Barrier-to-Autointegration Factor (BAF) phosphorylated at Thr2, Thr3, and Ser4 (circled in red) suggests that inhibition of DNA binding by phosphorylation is due to both steric clashes and destabilizing electrostatic interactions with the DNA phosphate backbone. The helix-hairpin-helix DNA binding motif is orange, the N-terminal fragment that interacts with DNA is yellow, and side chains of residues implicated in DNA binding are displayed.

Tim Umland, HWI and U. Buffalo, presented a beautiful poster, PT15, that reported on the 1.08Å structure of an evolutionarily conserved essential host factor called the Barrier to Autointegration Factor (BAF) protein.

This host protein is important for retrovirus and poxvirus replication. The structure was compared to a lower resolution structure with DNA and an NMR structure of a complex with the nuclear envelope protein Emerin. Refinement is still on-going, but the high resolution data gave additional information about the protein's multiple interaction surfaces and helped to explain the protein's lowered affinity for dsDNA; modeling of phosphorylated Ser/Thr residues showed likely steric and electrostatic clashes.

We encourage all members to remember that if your macromolecular structure work does not seem appropriate for a topic-related session, and even though your structure is not new or "cutting-edge," -your structure is "exciting" to you and will be "exciting " to many others; please submit such posters to the "Exciting Structures" session next year!

John Horton and Jack Tanner



Cartoon courtesy of Nick D. Kim, nearing-zero.net.

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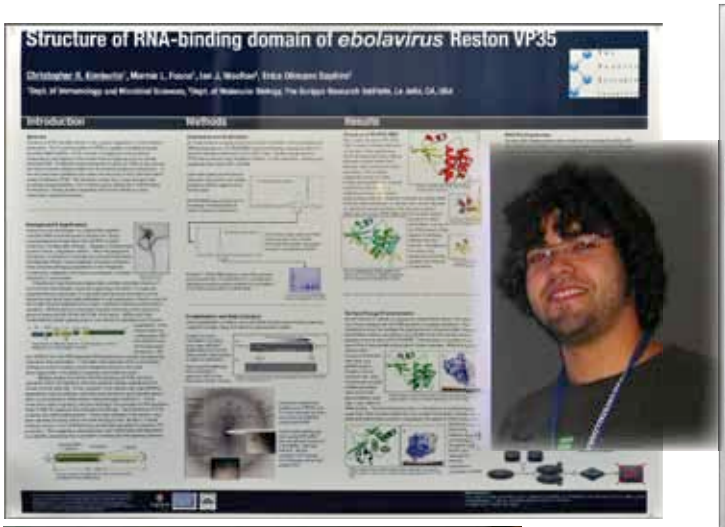
Judging for the 2009 Poster Awards was organized by Victor Young.

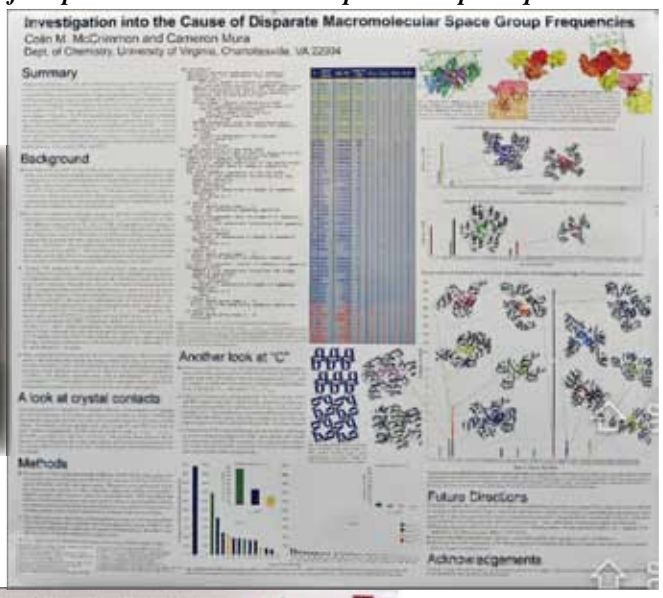
2009 Pauling Prizes

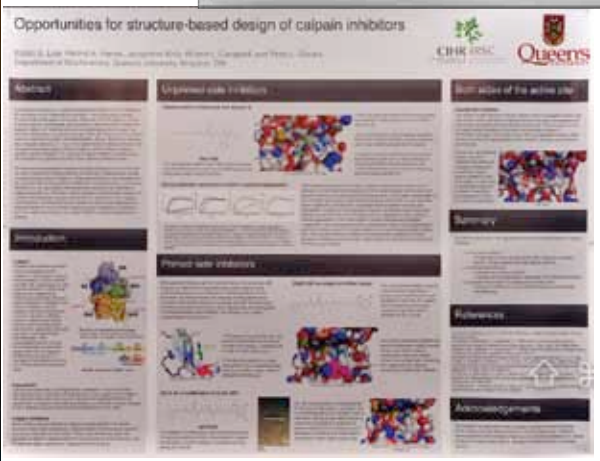
Pauling Prizes are awarded to the best student poster presentations at the ACA annual meeting. Each award consists of $200, a complementary banquet ticket, and a copy of Linus Paulings General Chemistry. Pauling judges this year were **Hilary Jenkins**, **Andreas Decken**, and **Frank Fronczek**.

The winning **Pauling Prize** poster was **PS041** by **Christopher Kimberlin**, Scripps Inst., for ***Structure of RNA-binding domain of ebolavirus Reston VP35.*** The **Canadian Pauling Prize**, awarded to the best Canadian student poster, went to **Kristin Low**, Queens U., Kingston, for **PM093**, ***Opportunities for structure-based design of Calpain inhibitors.***

The **IUCr Poster Prize** is awarded to the poster presented at the ACA annual meeting with the best look, content and presentation. For the 2009 award, the committee selected **Colin McCrimmon,** U. of Virginia for **PS009**, ***Investigation into the Cause of Disparate Macromolecular Space Group Frequencies.***





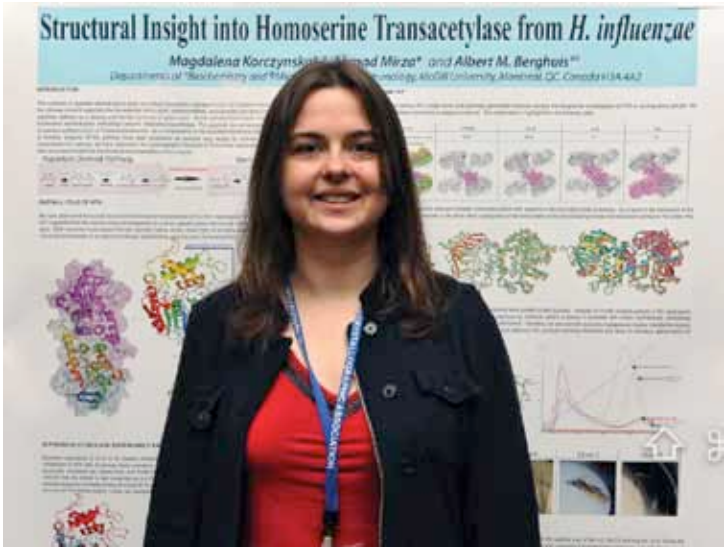


IUCr Pauling Prize. Above, **PS009**, the winning poster by **Colin McCrimmon**. Colin won the **AIP Undergraduate Prize** also, and is pictured on the next page.

Journal of Chemical Crystallography Prize

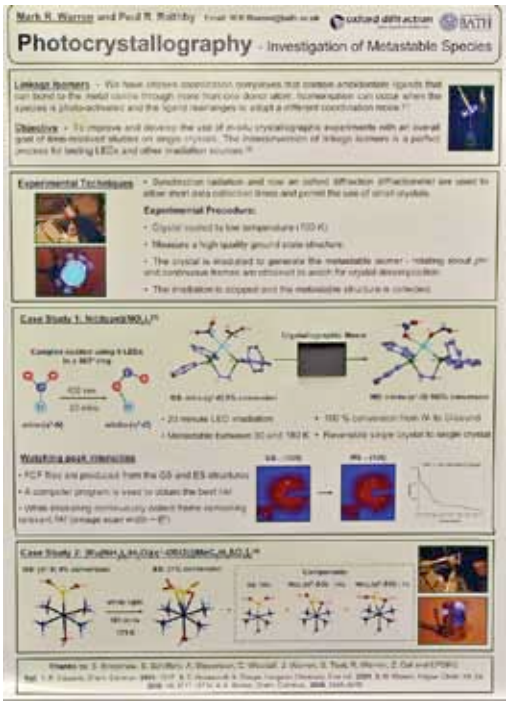
The **JCC Prize** is awarded to the best student poster presented at the ACA annual meeting in the areas of chemical crystallography or small molecule structure determination or analysis. For the 2009 prize, the JCC Prize Committee: **Carla Slebodnick**, **Amy Sarjeant**, **Danielle Gray**, and **Xiaoping Wang** selected **Britt Vanchura II**, for his poster **PM073**, ***Stable, 5-coordinate Trisboryl Analogs of Proposed Reactive Intermediates in Ir-Mediated C-H Borylations.***

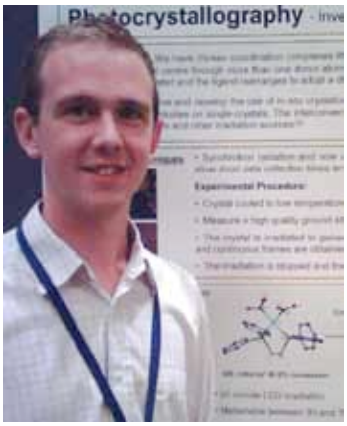
2009 RCSB Protein Data Bank Prize



Nobody expected it to be easy but the members of the selection committee for the RCSB PDB Poster prize, **Joe Ng**, **John Rose**, **Pawel Grochulski** and **Emil Pai** learned quickly that the very high quality and the sheer number of poster contributions posed a formidable challenge to judge. After a methodical screening by individual members, the full committee then interviewed the leading contenders asking them for the "condensed-to-5-min" version of their poster presentation. Her "Structural Insight into Homoserine Transacetylase from Haemophilus influenzae" put **Magdalena Korczynska,** McGill University, at the top of the list. She won the judges' thumbs-up not only with an excellent layout of her poster W0483 but also with her eloquent description of her analysis of the protein's dimer interface and the explanation of the importance of this enzyme as part of the methionine biosynthesis pathway with effects on protein synthesis and a variety of metabolic processes. The enzyme is essential for microbial organisms but absent in homologous pathways in humans, making it an attractive candidate for antimicrobial drug development.

Emil Pai





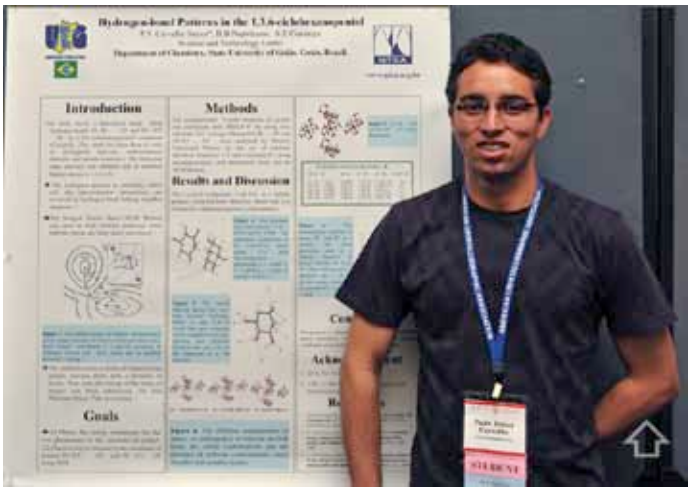
Oxford Cryosystems Prize

The **Oxford Cryosystems Prize** is awarded to the best poster presented at the ACA annual meeting in the area of low temperature crystallography. The 2009 Oxford Cryosystems Prize Committee, chaired by **David Rose**, **included Jim Rini, Marie Fraser**, **Pawel Grochulski,** and **Bill Furey**, selected **Mark Warren**, U. Bath, UK, for his presentation **PM068**, ***Photocrystallography - Investigation of Metastable Species.***

David Rose commented that in their reviews the committee stressed that they were looking for innovative use of cryo techniques - not just collecting data at low temperatures. Mark's poster described using temperatures to trap different chemical states in the crystal.

AIP Undergraduate Research Poster Prize

This prize is sponsored by the AIP through the Society of Physics Students; the student must demonstrate a command of the science, and must have completed the majority of the work; the winner receives $200 and a banquet ticket. The 2009 judging committee included **Henry Bellamy, Mark Wilson, & Chair, Bernhard Rupp.** The 2009 AIP undergraduate Prize was presented to two undergraduates, **Colin McCrimmon**, see preceding page because Colin also won the IUCr Pauling Prize, and to **Paulo Caravalho, Jr**., Michigan State U., **PM098**, for ***Hydrogen-bond Patterns in the 1,3,6-Cyclohexanopentols.***



Hosting ACA Summer Courses

Each ACA Summer Course is awarded to a specific site for a period of four years. Traditionally two Courses are offered, one on small molecule crystallography and the other on macromolecular crystallography, although applications for other topics are open for consideration. The Courses are held every year in the summer and should run for 10 to 12 days, with the dates not conflicting with any ACA or IUCr meetings. Applications to host must meet certain requirements and they should try to meet suggested guidelines. Check the ACA homepage for any late breaking changes or additional requirements beyond those provided here prior to proposal submission. Applications should indicate how all requirements and guidelines would be met.

Requirements: 1) The site should accommodate at least 20 students. Ideally classes should be comprised of 10 to 50 students. If student housing cannot be provided on-site, daily transportation must be provided.

2) The Courses must have a mix between theory lectures, demonstrations and hands-on training/exercises. For example 35% lectures, 15% demonstrations, and 50% hands-on training/exercises would be fine; other ratios might be acceptable. Theory lectures should precede any practical sessions dealing with application of that theory.

3) Students must have access to adequate computing facilities and diffraction equipment to allow for effective hands-on training. For the duration of the Course, the following equipment must be accessible to both Course students and faculty:

> At least one computer for every two students (ideally one for each).
>
> For small molecule Courses, at least one operational single crystal diffractometer equipped with an area detector and low-temperature device, and at least one operational powder diffractometer.
>
> For macromolecular Courses, access to a synchrotron and/or local access to several operational in-house protein crystallography data collection instruments (e.g. high-flux source, focusing optics, area detectors, low temperature devices, etc.)

4) Every student should personally mount and, when appropriate, cryoprotect and freeze a crystal. Each student should collect and process data, ideally from that crystal; for the **small molecule Course**, each student should be involved in performing data reduction and absorption corrections, solve and refine at least one structure, and run a powder sample. For the small molecule Course students should be encouraged to bring their own crystals; for the **macromolecule Course** students should be encouraged to bring their own samples for crystallization setups and crystallization should be included in the lectures and lab.

5) At the end of the Course, every student should fill out an evaluation form ranking course strengths, weaknesses, and whether or not the Course met their needs/expectations. The form should also include a field for suggested improvements. All forms should be collected and turned in promptly to the ACA with copies to the ACA's **Continuing Education Standing Committee.**

6) The prospective program plan should include a reasonably detailed budget, organizers / host organizations, a tentative list of instructors, tentative syllabus, scientific and housing facilities, expected costs, expected income raised from student fees, amount requested from the ACA, and amount expected to be raised through donations.

7) The organizer(s) of the Course must submit a written report to the ACA Standing Committee on Continuing Education (with a copy to the Buffalo Office) within 60 days of Course completion. This report should contain a summary of the Course, a list of student attendees with their home institutions, e-mail addresses, status (i.e. undergrad, grad student, postdoc, etc.), and which students, if any, received stipends. The report should also contain a breakdown of actual expenses by category and a list of participating faculty members present during the Course. It may also contain items of special mention (i.e. suggestions for improvements, exceptionally good results, etc.) as well as a list of any field trips or coordinated social activities.

Guidelines: 1) Organizers are encouraged to have a large faculty. Experienced crystallographers from all over the country and possibly abroad should be recruited. Some young faculty members who are actually doing crystallography in the lab might be invited, especially for the hands-on part. The Summer Course is a place for the students to network; being exposed to a large number of teachers is helpful for this aspect.

2) Time for socializing between students and between students and faculty is desirable. Lunchtime offers opportunities, as do some evenings ending not later than 9:00 p.m., perhaps followed by general, open discussions. A picnic on the Sunday is also an option. Contacts made at the Summer Course are as important as the knowledge taught.

3) At the last day of the Summer Course, every student should present a brief (~ five minutes) report to all students and faculty about his work at the Course. This obviously benefits both students and faculty. In recent years Charles Lake has done this successfully at the small molecule Courses.

4) Lecture hall, computing facilities and crystallization/diffraction labs should be located near to one another, synchrotrons being an exception if remote data collection is used. Students should ideally be housed within walking distance.

5) Ideally, faculty housing would be nearby too. Contacts with faculty are an important aspect of the ACA Summer Courses.

6) A diverse student body is desirable. Full scholarships for deserving students, as introduced by **Charles Lake**, should help increase diversity, e.g. students from South- and Central-America, and also from not-so-well-off domestic universities. The organizer should try to have as many students as possible receive partial or full scholarships.

7) While Course students certainly gain valuable training, if the lecture materials were also made available to the general public. e.g. via a website, the Course could benefit a significantly larger group of ACA members and others. **Andy Howard** has done this for the macromolecular Course the past few years, and in some years those lectures were also videotaped.

Bill Furey for the Continuing Ed Committee: Chris Cahill, Bill Furey, Peter Müller & Allen Hunter

Crystallography School at the UFMG – March 26, 2009 – Physics Department, Institute of Exact Sciences (ICEX), Pampulha Campus, UFMG, Belo Horizonte, MG - BRAZIL

Organizing Committee:

Carlos Basílio Pinheiro – Physics Department - UFMG (Coordinator)
Nelson Gonçalves Fernandes – Chemistry Department - UFMG
Nivaldo Lúcio Speziali – Physics Department - UFMG
Ronaldo Alves Pinto Nagem – Biochemistry Department - UFMG

Carlos B. Pinheiro and Nivaldo L. Speziali

The Federal University of Minas Gerais (UFMG) has a well known tradition in experimental research in different areas, many of which are greatly dependent on structural studies. For this reason, the creation of a new Center for the Structural Characterization of Materials and Molecules (CCEM&M) was a great occasion. To complete the facility of the Laboratório de Cristalografia (LabCri) new diffractometers dedicated to small molecule investigations have been acquired whereas a rotating anode dedicated to the studies of protein structures will be commissioned soon at the Biochemistry Department .

The audience: -more than 120 participants.

The lectures presented were preceded by an introduction on the multidisciplinary nature of crystallography (I.L. Torriani), followed by presentations on different subjects such as: structural crystallography at the UFMG (N.L. Speziali), characterization of supra-molecular compounds (R. Diniz), protein crystallography (J.A. Barbosa), study of thin films (M. Fantini), applications of XRD in metalurgy (V. Buono), applications of XRD in industry (F.Costa), polymorphism (J.Ellena) and XRD in nanocrystalline matrials (S.R. Teixeira)..

This was a very successful meeting. The organizers reached the right interested groups, and a lot of activity is expected from the UFMG experienced researchers and young students in the near future

Iris L. Torriani

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Meeting website: http://meeting2010.AmerCrystalAssn.org/

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Transactions Symposium
The First Element, a symposium to honor the memory of Bob Bau, chemist, diffractionist, neutron scattering expert and promoter, with special focus on the future of studies involving hydrogen.
Chairs: Christine Hoffman, Larry Falvello, Thomas Proffen, Nobuo Niimura.

Trueblood Award to Anthony L. Spek

Etter Early Career Award to Raymond Trievel,

Etter Award Symposium Chair: Ryan Jackson
-sponsored by General Interest & YS-SIGs.

Award Symposium or Plenary Lectures every day. The workshops are not yet set as we go to press in mid-September. See the meeting website for an update.

All photos, and ACA Logo from Bernie Santarsiero

NOVEMBER 2009

9-10 Protein Science Forum, De Vere- Wokefield Park Hotel, Goodboys Lane, Mortimer, Reading, Berkshire, RG7 3AH, UK.

FEBRUARY 2010

15-18 Biology and Synchrotron Radiation (BSR) and Medical Applications of Synchrotron Radiation (MASR), Melbourne, Australia. **http://www.bsr2010.org/**.

MARCH 2010

21-25 Spring ACS National Meeting & Exposition, San Francisco, CA

JUNE 2010

6-11 **Gordon Research Conference in Crystal Engineering,** Waterville Valley Resort, Waterville Valley, NH **www.grc.org/programs.aspx?year=2010&program=crystaleng.**

JULY 2010

24-29 **ACA2010, Chicago, IL. Local chair: Bernie Santarsiero (bds@uic.edu); Program chair: Ross Angel (rangel@vt.edu). See page 51.**

18-23 **Gordon Conference on Diffraction Methods in Structural Biology,** Bates College, Lewiston, ME. **www.grc.org/programs.aspx?year=2010&program=diffrac.**

AUGUST 2010

29-2 ECM26, European Crystallographic Association Meeting in Darmstadt, Germany.

29-3 EUCMOS 2010, European Conference on Molecular Spectroscopy, Florence, Italy. **http://www.unifi.it/eucmos2010**.

SEPTEMBER 2010

12-16 13th ICCBM, Crystallization Workshop, Trinity College, Dublin, Ireland. **www.iccbm13.ie**.

MAY 2011

21-26 **ACA 2011, Sheraton Hotel New Orleans, New Orleans, LA. Program Chair: Chris Cahill; Local Chairs: Cheryl Klein-Stevens & Ed Stevens.**

AUGUST 2011

22-29 **XXII Congress and General Assembly of the IUCr.** Madrid, Spain. **www.iucr2011madrid.es.**

JULY 2012

28-2 **ACA2012, Westin Boston Waterfront Hotel, Boston, MA.**

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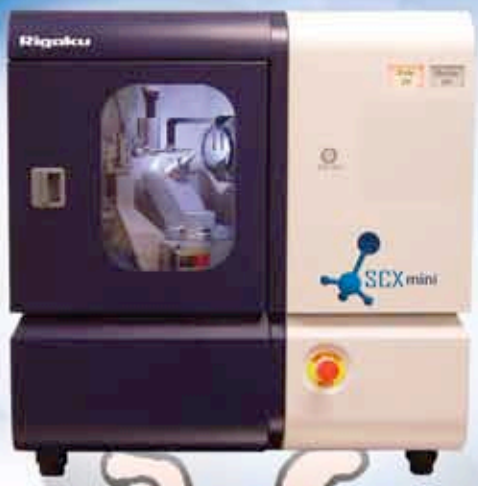

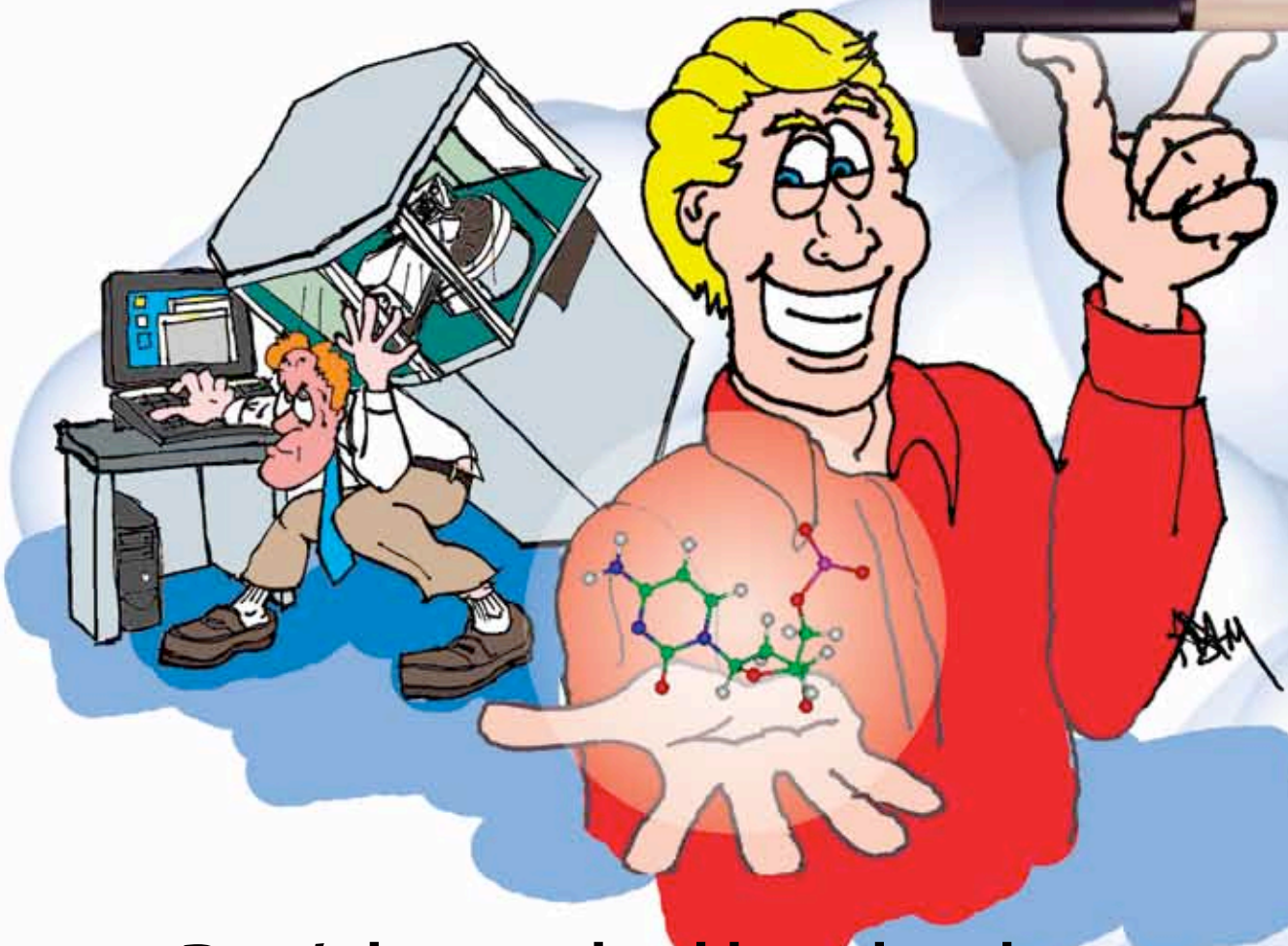

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