

INTERNATIONAL UNION OF CRYSTALLOGRAPHY

IUCr Newsletter

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Original article text and available illustrations

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LETTER FROM THE PRESIDENT

Letter from the President



William L. Duax

It is a pleasure and an honor to have been elected to serve the crystallographic community as President of the IUCr. Now, more than at any other time in history, it is important that we set aside national interests and embrace the principles of the International Union. Those principles include free circulation of scientists, education of the new generation of scientists everywhere, and assistance to emerging nations. Emerging nations can benefit from the use of the powerful techniques of X-ray crystallography in order to analyze, understand and use the unique natural resources within their countries whether mineralogical, chemical, or biological in nature.

It is noteworthy that the Union consistently uses its financial resources to support countries in need and students everywhere. I urge you to support all of the activities of the IUCr. Consider publishing some of your best work in *Acta* or starting a personal subscription to an *Acta* Journal. Establish a collaboration with a research scientist on another continent in order to advance science and support international communication. Consider volunteering to assist one of the Commissions of the Union in achieving its objectives. If you have ideas, concerns or opinions about the activities of a Commission of the Union, please express them. If you think that there are areas vital to crystallography and crystallographers that might be served by a new commission, a new publication, or a new volume of the International Tables, address your ideas to me or the individuals you consider best qualified to evaluate and implement your requests.

The Regional Affiliates of the IUCr have become powerful resources to advance the goals and principles of the Union. The European Crystallographic Assn has a vital African Initiative, the American Crystallographic Assn has a Latin American initiative and the more advanced countries in the Asian Crystallographic Assn are helping to strengthen crystallography in their region. When you travel to another country, consider yourself an ambassador for crystallography. Contact crystallographers in the cities you visit and find out what they are doing and, where appropriate and feasible, offer your support and assistance. This is especially important if you visit a country that is not now a member of the Union. Presently, 38 countries are members of the IUCr and are listed on the IUCr website. Other international scientific societies have membership of as many as 90 countries. Many of these other countries would benefit from IUCr membership. The easiest way to spread the word about the IUCr is to have the IUCr Newsletter distributed to individuals who may be interested in crystallography and science libraries in nonmember countries. If you have friends, colleagues, or collaborate in countries that are not now members of the IUCr, please send these names and address to the IUCr office so that they can be added to the mailing list.

Perhaps the best thing each of you could do for yourself, your science and others would be to volunteer for a leadership role in a scientific organization, work for international cooperation, and encourage young people to become involved.

Bill Duax

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EDITORIAL

Editorial



2003 promises to be a year of new beginnings and exciting challenges for me. On a personal note I have left the Naval Research Laboratory to take a position with the Protein Data Bank (PDB) - quite a leap for a dyed-in-the-wool small molecule crystallographer. Even from the small molecule perspective I have always viewed the PDB as a critical international resource. I am pleased to be joining the team responsible for its maintenance and growth.

My second new beginning is that I am one of the new coeditors of *Acta Cryst Section E*. In this capacity I look forward to maintaining ties with my colleagues in the structural chemistry community.

And last, but not least, the IUCr Newsletter will be new for me in 2003. Unlike the ACA Newsletter, whose editorial duties I share with Connie Chidester, this publication has a strict page limit. Therefore, the 'edit' in editor has real meaning here. When an article is submitted that is too long for the Newsletter it must be shortened. Since it is often difficult for someone not directly involved to know which parts of the article are most important, please keep brevity in mind when you submit material for publication. The author should know far better than the editor what the salient highlights of the meeting or story are. And don't forget, a (high resolution) picture is worth a thousand words.

I think that Bill has done a fantastic job with the Newsletter over the past 10 years so I plan to continue using the model he has developed. We would like to print a variety of news of interest to our community (IUCr Commission activities, what's happening in the various crystallographic associations, election results, awards, obituaries, book reviews, letters to the editor, relevant web-sites, future meeting announcements, new resources, etc). Please continue to submit articles you feel would be of interest to our readers. Bill published just about everything that was submitted to him and I hope to be able to do the same.

I look forward to working with all of you.

Judy Flippen-Anderson
flippen@rcsb.rutgers.edu

LETTER TO THE EDITOR

A personal definition of crystallography

Dear Editor,

I have noted from the *IUCr Newsletter* (Vol. 10, No. 2) that *Z. f. Krist.* would publish a 'personal definition of Crystallography'. Unfortunately, I was late in submitting the paper and hope that my definition can be announced at your periodical:

'Crystallography is the science concerned with reasons, laws, and consequences of space ordering of atoms, atomic groups (molecules, clusters, etc.), and, generally, a great deal of identical material objects of the one or several sorts'.

S.V. Borisov

IUCR JOURNALS NEWS

Can a multipole analysis faithfully reproduce topological descriptors of a total charge density?

***Acta Cryst.* (2002). A58, 451-459**

Ian Bytheway, Graham S. Chandler and Brian N. Figgis

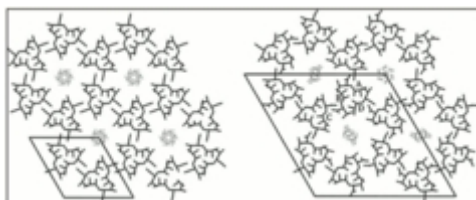
Using a multipole expansion to extract a charge-density distribution from X-ray data is known to show disagreement with theoretical calculations of the same density. The origin of these differences has been attributed to various causes. This paper examines the accuracy of the multipole fitting itself by starting from a precisely known density for crystalline ammonia. This charge density is transformed into thermal-motion-free structure factors, which are then fitted using the usual techniques of multipole analysis.

Through topological analysis it is shown that, except for the Laplacian of the density, agreement to better than 12% can be achieved for the topological parameters. The goodness-of-fit factor and residual plots show that the multipole refinement strategies used are far from perfect, although, when thermal motion refinement is included, they do sample the experimental structure factors of Boese *et al.* [*J. Phys. Chem.* (1997). B**101**, 5794–5799] extremely well.

An exceptionally stable peptide nanotube system with flexible pores

***Acta Cryst.* (2002). B58, 849-854**

Carl Henrik Görbitz



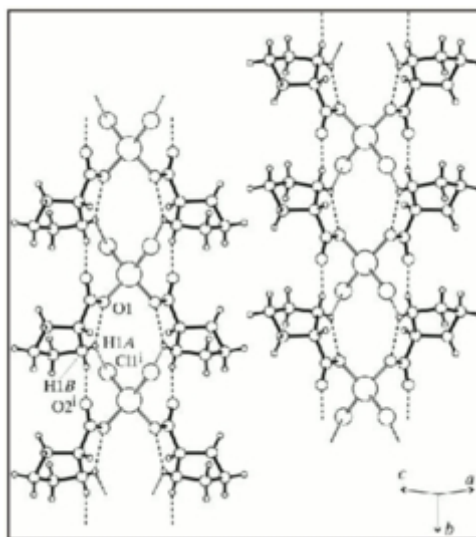
The unit cell and molecular packing of $\text{C}_8\text{H}_{16}\text{N}_2\text{O}_3 \cdot 0.35\text{C}_2\text{H}_3\text{N}$ (left) and $\text{C}_8\text{H}_{16}\text{N}_2\text{O}_3 \cdot 0.25\text{C}_3\text{H}_8\text{O} \cdot 0.22\text{H}_2\text{O}$ (right) viewed along the c axis. Solvent guest molecules are shown in grey, positions for water molecules in $\text{C}_8\text{H}_{16}\text{N}_2\text{O}_3 \cdot 0.25\text{C}_3\text{H}_8\text{O} \cdot 0.22\text{H}_2\text{O}$ appear as small crosses. In a series of data collections on a selected single crystal of the dipeptide L-Ala-L-Val, space group $P6_1$, it is shown that small guest molecules like acetonitrile, methanol and acetone can be removed from hydrophobic channels parallel to the hexagonal axis without impairing the structure of the hydrogen-bonded peptide host structure. L-Ala-L-Val is one of the very first organic molecules with this property. Alcohol guests larger than methanol are also absorbed, but they induce a doubling of the a and b axes as well as a change in the shape and size of the pores. The observed structural modifications explain why these solvent molecules are more or less irreversibly trapped inside the channels.

IUCR ACTIVITIES

Dichlorobis(DL-proline-κO)zinc(II)

***Acta Cryst.* (2003). C59, m18-m20**

Martin Lutz and Ruud Bakker



Hydrogen-bond formation in the crystal structure. The proline residues in the chain on the left-hand side have the *R* configuration, while those on the right-hand side have the *S* configuration [symmetry code: (i) $x, 1 + y, z$].

Neutral, zwitterionic amino acids form adducts (neutral salts) with metal salts like LiCl, CaCl₂ or ZnCl₂. Thereby the negatively charged carboxylate group binds to the cation of the salt, and in most cases the positively charged ammonium group donates hydrogen bonds to the anions. This paper reports on the neutral salt of DL-proline with ZnCl₂. The Zn cation is tetrahedrally four-coordinated with two chlorine anions and two proline residues as ligands. Because the Zn is located on a twofold axis, these two proline residues have the same absolute configuration. By hydrogen bonding infinite linear chains of these molecules are formed, consisting of molecules with the same chirality (partial separation of enantiomers). Due to the centrosymmetry of the space group, the same amount of *R* and *S* chains is present in the crystal. Under different crystallization conditions a complete separation of the enantiomers was observed, resulting in a crystalline powder of the enantiopure compounds.

IUCR JOURNALS NEWS

PHENIX: building new software for automated crystallographic structure determination

***Acta Cryst.* (2002). D58, 1948-1954**

Paul D. Adams, Ralf W. Grosse-Kunstleve, Li-Wei Hung, Thomas R. Ioerger, Airlie J. McCoy, Nigel W. Moriarty, Randy J. Read, James C. Sacchettini, Nicholas K. Sauter and Thomas C. Terwilliger

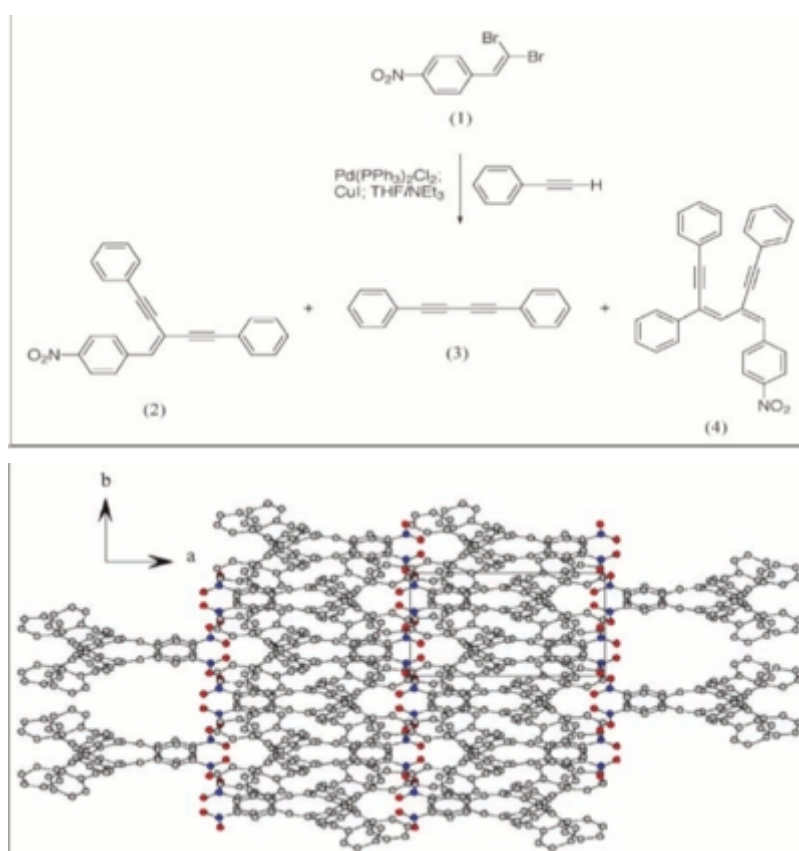
The PHENIX software, a new open system for automated crystallography, is described. The software is based on modern computational concepts and tools including object-oriented programming and the Python high-level scripting language. This architecture, in combination with a sophisticated graphical environment, allows users to rapidly develop complex algorithms interactively without the need for time-consuming programming. Software developers can use the same infrastructure to integrate new software into the system. PHENIX also makes use of distributed computing and automated data management, features important for high-throughput crystallography. Many of the components of the system are general and can easily be applied to other areas of structural biology.

π - π -Stacking and nitro- π -stacking interactions of 1-(4-nitrophenyl)-4-phenyl-2,4-bis(phenylethynyl)butadiene

π - π -Stacking and nitro- π -stacking interactions of 1-(4-nitrophenyl)-4-phenyl-2,4-bis(phenylethynyl)butadiene

Acta Cryst. (2003). E59, o227-o229

Bilal R. Kaafarani, Brigitte Wex, Allen G. Oliver, Jeanette A. Krause Bauer and Douglas C. Neckers



The X-ray structure and stacking of 1-(4-nitrophenyl)-4-phenyl-2,4-bis(phenylethynyl)butadiene (4) is reported. This compound is a side product observed during the Sonogashira coupling reaction of β , β -dibromo-p-nitrostyrene (1) and phenylacetylene to afford β , β -bis(phenylethynyl)-4-nitrostyrene (2), a Y-enyne. Diynes, formed by reductive elimination, are classical side products in the course of the Sonogashira coupling reaction, in this case 1,4-diphenylbutadiyne (3). To the best of our knowledge, this is the first report of such a side product in the Sonogashira reaction. The nitro substitution induced π - π -stacking and nitro- π interactions in (4). The distance between the centroids of the phenyl rings in (4) alternates between 4.96 and 5.35 Å. The distance between the centers of the acetylene triple bonds is 3.28 Å. The scanning electron micrograph of (4) shows its crystal habit in the form of complex, cactus-like needles with a diameter of several micrometers.

MEETING REPORT

Crystallography at high pressure

Orsay, France, September 4-9, 2001

Participants at the Crystallography at High Pressure - 2001 international workshop in Orsay, France. This international workshop was organized by the IUCr Commission on High Pressure. The French national neutron facility, Lab. Léon Brillouin, served as the host organization. The Commission determined the scope of the meeting and provided most of the suggestions for the scientific program. I. Goncharenko was chair of the Organizing Committee and R. Nelmes chaired the Program Committee. In each triennium the Commission holds one meeting that covers the full scope of its activities: structures and transitions, new materials, Earth and planetary sciences, soft and biological matter, physical and chemical properties, theory and computation, and technique developments on synchrotron, neutron and laboratory-based facilities. Special efforts were extended to bring new names into the program. Many of the invited speakers and most of the invited poster orals presenters were young researchers, postdocs or PhD students.

We would like to thank members of the Organizing Committee, J.-M. Mignot (vice-chair), I. Mirebeau and P. Cadavez-Peres. The meeting would not have been as successful as it was without the efforts of O. Makarova, B. Mailleret, C. Pomeau, C. Rousse, I. Rault, F. Berger, J.-P. Itié and A. Polian. The IUCr, CEA (French Commissariat of Atomic Energy), CNRS (French Nat'l Centre for Scientific Research) and the French Ministry of Research all contributed to funding of the Workshop. These funds allowed support for more than 30 young scientists.

At a session devoted to soft and biological matter the audience learned about a structural basis for pressure effects in proteins from P. Urayama, and exciting recent progress in structural refinement of diamond-anvil-cell data from proteins presented by R. Fourme, and enjoyed a well illustrated talk from R. Templer on lyotropic phase transitions induced by pressure jumps. W. Poon used all his artistic talents to describe a brilliant future for studies of protein dynamics and A. Lefebvre described nucleation in polymers under pressure. Two poster orals, presented by G. Pépy and I. Ascone, highlighted results obtained on neutron and soft x-ray facilities.

The program continued with studies of liquid and amorphous systems. Mohamed Mezouar highlighted recent developments at the ID30 beam line (ESRF) for studying liquids under high P-T conditions. C. Benmore outlined some advantages of neutron techniques (H/D contrast) in studies of critical and sub-critical liquids. The invited talks were supplemented by a poster oral on pressure driven amorphization (D. Machon).

The program then turned to crystal structures and phase transitions. Progress in *ab-initio* calculations of crystal structures and physical properties was overviewed by B. Winkler. M. McMahon presented new results on several remarkably 'weird' structures occurring in simple metals under high pressures. In another theoretical talk, J. Dong predicted new crystal structures in solidified gases. P. Dera described experimental studies of H-bonding materials. Various aspects of structural transitions in cristobalites and titanites were described by J. Haines and S. Rath.

One session was devoted to the late Jean-Michel Besson ('Michel' to his friends and colleagues), who was a mentor, friend or collaborator for many of the participants in the Workshop. Michel made exceptional contributions to modern high-pressure science, especially in recent times by developing the Paris-

Edinburgh pressure cell. He will long be remembered for his remarkable activity and enthusiasm. The talks in this session were given by Michel's ex-colleagues or students: A. Polian, P. Loubeyre, S. Klotz, and Y. Le Godec. Their talks covered Michel's many seminal contributions to high-pressure science, with highlights taken from studies of light elements under pressure, neutron results on high-density amorphous ice and progress in high P-T neutron diffraction. The session was introduced and chaired by R. Nelmes.

At the session on magnetic crystallography P. Cadavez-Peres, Kenji Ohwada, J.-M. Mignot and A.-K. Klehe emphasized highly unusual physical phenomena in magnetically unstable compounds, spin-ladders, intermediate valence systems, and organic superconductors under high pressure. The experimental methods ranged from neutron and x-ray diffraction to optical spectroscopy. All the speakers managed to keep their talks (involving rather 'heavy' physics) lively and understandable. N. Kernavanois and A. Hannan complemented the oral talks by presenting poster orals on recent advances in resonant x-ray scattering at the ESRF and neutron diffraction under pressure at the Japanese neutron facility JAERI.

Rapid developments in the studies of ices and hydrates were illustrated in talks by W. Kuhs on intercalation of noble gases in ices, by H. Itoh on molecular dynamics simulations in hydrates, and by J. Loveday on conditions for the formation of new methane hydrates probably occurring in Saturn's moon, Titan. In a poster oral, S. Desgreniers covered recent x-ray results on silicon and analogous water clathrates.

In the session dedicated to new technical developments O. Shimomura described recent high-pressure activities on several beam lines at SPring-8. R. Hemley gave a talk on new types of anvil-cell (synthetic diamond, moissanite, etc.) which promise to expand the limits for available volumes and maximum pressures in x-ray and neutron studies. D. Keen presented a poster oral on recent progress in high-pressure single-crystal neutron diffraction at ISIS.

Recent progress in inelastic x-ray scattering in geophysical materials under pressure was described by G. Fiquet, a possible scenario for chemical reactions in the giant planets was proposed by R. Benedetti, and studies of Fe-O systems at the Earth's lower mantle conditions were presented by L. Dubrovinsky. A talk on theoretical aspects of the Fe-S system under the conditions of the Mars interior by P. Martin was complemented by a poster oral on experimental studies of the same system by C. Sanloup.

A number of talks focused on inelastic studies and techniques. J. Tse discussed phonons and structural transformation in solids. W. Sturhahn and R. Hemley spoke on nuclear resonant and inelastic x-ray studies at the APS and the BNL. M. Braden and D. Kozlenko described progress in inelastic neutron scattering at the LLB and IBR-2. The exclusivity of neutron techniques in providing detailed information on dispersion curves under pressure was questioned by a poster oral on inelastic single-crystal x-ray scattering from F. Occelli. There were also visits to the neutron (LLB) and synchrotron (LURE) sources located near the conference venue. The participants had guided tours through the facilities and high-pressure installations, and we thank M. Braden, J.-P. Itié and L. Noriez who acted as guides.

In a session on new materials and high-pressure synthesis R. Ahuja spoke on a new high-pressure phase of TiO_2 and V. Solozhenko presented recent results on ternary C-B-N alloys. Both compounds are believed to be among the hardest known materials but possibly they will not resist polymerized C_6O ! N. Serebryanaya (poster oral) claimed that this new phase formed from C_6O can scratch a diamond. E. Soignard presented new results in high-pressure nitrides and A. San-Miguel spoke on EXAFS and x-ray studies of silicon clathrates.

Quasiperiodic and nanomaterials were represented by A. Sadoc and T. Watanuki who gave intriguing examples of x-ray and EXAFS studies of quasicrystals. S. Rols and S. Sharma described structural changes and superelastic properties of carbon nanotubes studied by neutron and x-ray diffraction, respectively.

The workshop ended on the topic of physical properties. K. Shimizu presented striking data on pressure-induced superconductivity in elementary iron. A. Huxley spoke on the co-existence of magnetism and superconductivity in the UGe_2 compound under pressure. E. Pugh gave a poster oral on quantum critical behavior in Sr_2RuO_4 . M. Abd-Elmeguid ended the workshop with a lively talk on structural instability versus magnetic and electronic instabilities in Eu-phosphides.

Best poster presentations went to C. Sanloup (first) for her poster on Fe-S liquid alloys, and to N. Serebryanaya for her poster on polymerised C_6O phases and T. Watanuki for his poster on quasicrystals (tied for second).

Igor Goncharenko and Richard Nelves

MEETING REPORT

XIX Congress and General Assembly



'...The original venue for IUCr XIX was Jerusalem - often connoted the 'City of Peace'. Throughout its history, however, Jerusalem, the meeting point of three continents and the focus of three religions has witnessed periods of conflict. Unfortunately, we are living through one of these periods. So, in May of 2001 we moved the venue of IUCr XIX from the City of Peace here to Geneva, a city which prides itself on being a place where in the past peace has been made among nations and making peace for the future is a business of the present.

We are reaching the end of another rather long and varied scientific meeting, during which we have enjoyed the sharing of ideas and the collegiality of fellow scientists. They came from more than fifty countries and a variety of cultures and backgrounds. Some might argue that a scientific meeting is a luxury of peace; others, that it serves to promote the peace we all long for. I would like to toast all the participants in IUCr XIX who came to Geneva to participate in this meeting and wish them godspeed in their return in peace to their homes and laboratories with renewed scientific enthusiasm and deepened friendship, to meet again in this forum in Florence in 2005. Bon Appetit, a pleasant evening - LaChaim.'

Joel Bernstein at the Congress Banquet

Keynote reports

New superconductor MgB_2 and related compounds



Jun Akimitsu and Evgeny Antipov

J. Akimitsu (Aoyama-Gakuin U., Japan) described the structure, effects of substitution and physical properties of this superconductor exhibiting the highest T_c (39K) among metal and alloys. The discovery of superconductivity in MgB_2 by J. Akimitsu and co-workers in January 2001 was one of the most important achievements in Solid State Physics and attracted great attention in the scientific community resulting in a large number of publications (about 1.5 citations per day).

Evgeny Antipov

The good, the bad and the ugly; experiences at the synchrotron



E. Garman and Z. Dauter

Z. Dauter (NCI, Brookhaven Nat'l Lab, USA) described the use of synchrotron radiation for structural biology. He outlined the essential components of a protein crystallography beamline, showing examples from beamline X9B at BNL, where he is coordinating an effort to integrate diffraction data collection and processing into a single control programme. He showed some potential pitfalls of synchrotron data collection, including the undesirable effects of radiation damage, but much to the relief of the audience, he did not categorise his many beamline users into 'Good, Bad or Ugly'!

The questions and comments at the end of the lecture focussed on issues related to worldwide efforts to automate protein crystallography synchrotron beamlines, and how data quality might be affected by reduced experimenter intervention.

Elspeth Garman

Structural mechanisms of self-assembly and polymorphic supercoiling of the bacterial flagellum

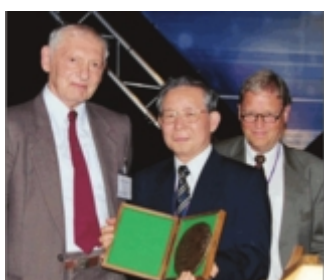


David Stuart and Carl Branden

K. Namba (Osaka U., Japan) reported on the simultaneous application of X-ray crystallographic, electron microscopic and other biophysical techniques in conjunction with biochemical and molecular biology approaches to unravel the structure and function of a nanomachine in the form of the bacterial flagellum which enables bacteria to swim. Although the flagellar filament is made up of a single protein flagellin, the tubular organisation of the protein molecules within it is such as to permit different modes of swimming. The motor at the base of the filament is connected to the latter by a hook which serves as a universal joint. Detailed structure analysis of the component proteins and their organisation in the flagellum have provided valuable insights into the complex movements that contribute to the mobility of bacteria.

M. Vijayan

Virus structure: the simple, the complex and the greasy



Michiyoshi Tanaka and Henk Shenk present Michael Woolfson with the Ewald Prize at the Opening Ceremony

D. Stuart (Wellcome Trust Center for Human Genetics, UK) focused on spherical viruses with emphasis on those that he and his group have studied in Oxford. The importance of quasi-equivalence for building up

the icosahedral viral coat was exemplified by the simple T=3 plant viruses which contain three identical subunits in the icosahedral asymmetric unit. Stuart pointed out that the same principle applies to the foot-and-mouth disease virus, FMDV, where the shell is built up from three chemically different but structurally similar polypeptide chains.

He also pointed out that the receptor binding site is quite different in FMDV from that in the related common cold virus.

Complex viruses were exemplified by the structure of the core of the bluetongue virus which his group determined a few years ago in a crystallographic 'tour de force' operation. The shell comprises 900 subunits of two different types. One type forms an inner scaffold in a T=2 arrangement which forms a symmetry mismatch to the T=13 outer layer formed by the second type of subunit. Nature overcomes the 'forbidden' T=2 arrangement by forming dimers with the subunits in different conformations. An animated display illustrated beautifully this arrangement. The transcription complex is inside the shell together with a high concentration of mRNA molecules, 400mg/ml. This RNA is highly organized by the scaffold.

The greasy viruses were exemplified by the bacteriophage PRD1 in which the core is enveloped by a lipid bilayer containing spike proteins. He also gave a progress report on his structural studies of a modified virus without the spike proteins which are done in collaboration with D.H. Bamford in Finland and R. Burnett in US. The crystals, which contain about 66MDa in the asymmetric unit, are unstable, diffract to 4Å resolution and give only one image per crystal. So far, 2,317,561 reflexions have been measured, phases were obtained from a cryoEM model combined with the known structure of one subunit and chain tracing is under way aided by the presence of 3,600 Se-met residues. He described features of the preliminary model and pointed out 150Å long thin strings of additional electron density running between the building blocks of the shell which corresponds to a 9kDa cementing particle called P30. He also showed electron density corresponding to the lipid bilayer where some structural organization could be seen. The structural studies of PRD1 which provide proof of principle that it is possible to obtain structures of enveloped viruses left the audience stunned in admiration.

Carl Branden

Contribution of direct methods to macromolecular structure determination

G. Sheldrick's (Göttingen, Germany) lecture, which played to a near capacity crowd on the last morning of the conference, displayed a neat symmetry with the opening lecture of the Congress given by M. Woolfson. In his Ewald Prize oration Prof. Woolfson, traced the development of direct methods from their early beginnings to their present use, which has extended to small proteins and more importantly as a combined approach with other methods to phase macromolecular structures. George Sheldrick took the liberty of redefining the title of his lecture to include not only *ab initio* methods but also the use of weak phasing information such as that which results from the anomalous signal from sulfur atoms in proteins or phosphorus atoms in nucleic acids. He outlined the dual real space/reciprocal space recycling methods implemented in *SHELXD* for both substructure solution and MAD phasing. An example included the location of 160 selenium atoms. *SHELXE* is the latest development in the *SHELX* family. It implements 'high throughput phasing' as a means to simply and quickly obtain robust phase information with a view to providing information at the time of data collection which can be used to further plan the conduct of the experiment. Despite the fact that *SHELXE* was not aimed at providing the final phases, in several cases it appears to be competitive with more sophisticated methods. It makes some simplifying assumptions including acceptance of the heavy atom coordinates from *SHELXD* without further refinement and the presence of only one type of anomalous scatterer. *SHELXE* also implements 'sphere of influence' density modification for more rapid calculation. In summary Prof. Sheldrick demonstrated that, despite his protestations that *SHELX* is only a hobby, he is playing a vital role in developing new

methods of structure solution and making them available to the community in a useable form. The lecture concluded with a discussion period.

Mitchell Guss

Chemical bonding as electronic coherence

W. Weyrich (U. of Konstanz, Germany) demonstrated with examples how the information from diffraction and Compton scattering studies can be combined using the Density Matrix (DM) representation of the electronic wave-functions in solids. He presented diagrams showing the relations of the observables in position and momentum space emphasizing that the chemical bonding cannot be understood by the charge density only, which corresponds to the diagonal part of the DM. The off-diagonal part carries essential information about the wave-function coherence between atoms, and this can be derived from the electron momentum density measured by Compton scattering (see abstract p. C191, *Acta Cryst. A* **58** (suppl.)).

There were several questions and comments from the audience:

Q: The negative parts in the Wigner function are not due to the Pauli principle, but rather due to the fact that the Wigner function is not a true phase-space density.

A: It is the Pauli principle that forces the electrons of the fluorine atom and molecule into *p*-orbitals, which give a negative contribution to the Wigner function. We agree about the non-classical nature of the Wigner function.

Q: Can it be expected that the approach of utilizing position and momentum densities for a more complete understanding of chemical bonding will be applicable to complex systems such as macromolecules, or will we have to extrapolate from findings for simple systems?

A: Since the momentum space data are vector-space data, they behave in a way similar to the Patterson function, though at the wave-function level rather than at the density level. I am therefore afraid that for very complicated systems we will have to extrapolate from simpler systems. Remember, however, that the essential information of chemical bonding in the diffraction data is included in a small number of low-order reflections. It can be envisaged that a comparable number of Compton profiles can be measured.

Q: Why are you so puristic and do not impose additional constraints such as a model on your reconstruction of density matrices?

A: By choosing a particular discrete representation, i.e. a basis set, we also have a model aspect. However, by a prudent choice we can come close to our goal of not biasing the result and rather following a clear, quantum-mechanically well-defined method.

P. Suortti

The GTPase switch: a familiar, conserved module with unexpected variations

A. Wittinghofer (MPI, Germany) began with an overview of the ever-growing number of branches of the Ras superfamily of GTP-binding proteins and their common functional cycle, which takes them from a GDP-bound or 'off' state to a GTP-bound or 'on' state and back again. These transitions are accelerated by guanine nucleotide exchange factors (GEFs) and GTPase activating proteins (GAPs), respectively, and only the triphosphate complexes interact with downstream effector molecules. The related structural characteristics were described, followed by examples of crystal structures of complexes between small G-proteins with their respective GEF or GAP. Although the core features, most of which can even be found in motor proteins, are repeated in all G-proteins, there still exists a wide variety of molecule-specific variations that contribute to the unique interactions typical for each G-protein. In contrast to the

conservation shown by the G-proteins, their GEFs and GAPs are completely unrelated; e.g. the RanGEF (RCC1) adopts a beta-propeller fold whereas the RhoGEF (Sos1) consists of mostly alpha helices; similarly, RanGAP, which contains 11 leucine-rich repeats that adopt the nonglobular shape of a crescent, bears no resemblance to RhoGAP or RasGAP. Despite their dissimilarity, GEFs and GAPs bind close to the 'switch regions' of the G- proteins. The interaction sites of the various effector molecules, however, cover almost the complete surface of the different G-proteins. Then, Dr. Wittinghofer discussed the roles of the members of the Rho branch of the family tree in the organization of the actin cytoskeleton, followed by striking examples of how various pathogens make use of this system in their quest to invade their host cells and exploit them to their advantage. The bacterial proteins involved are excellent mimics of their eukaryotic counterparts even at the mechanistic level but, again, structurally completely unrelated, which points to their independent origin and convergent evolution.

Emil F. Pai

COMCIFS open meeting

How to provide a seamless flow of computer-based information between crystallography and its neighboring disciplines was the question discussed during the open COMCIFS meeting held during the IUCr Congress in Geneva. The talks addressed the need for compatibility at the level of the definition of scientific concepts and at the level of file structures.

The session opened with a talk by B. McMahon and ended with a talk by J. Westbrook, both of whom pointed out the need for compatibility between the scientific definitions (the ontologies) provided by the CIF (Crystallographic Information File) dictionaries and those provided by the dictionaries of the disciplines of chemistry and biology. The Protein Data Bank has achieved a seamless connection with molecular biology by ensuring that the neighboring fields use STAR dictionaries that are fully compatible with CIF. Chemical databases are still in an experimental state and there is a danger that a variety of different and mutually incompatible dictionaries will be developed making it difficult to transfer information from one chemical data file to another and complicate the interchange of information between chemical and crystallographic databases.

The remaining talks of the session were devoted to compatibility of the file structures. While CIF has the best developed set of dictionaries of any discipline, it is currently not well provided with the software required to manipulate the files.

Disciplines now developing file structures are attracted by XML (eXtended Markup Language) because it is well provided with software written by the information technology community. However, few disciplines have developed the dictionaries needed for serious XML applications. Both J. Westbrook and N. Spadaccini described programs that can convert CIFs to XML files thereby allowing crystallographers to exploit the XML software, H. Bernstein showed that although CIF and XML have many similarities, there is more than one way in which a CIF can be mapped into XML. Emphasizing that CIF has always remained one step ahead of XML in functionality, S. Hall demonstrated an advanced dictionary language, StarDDL (Star Dictionary Definition Language), that will allow derived information to be calculated directly using algorithms stored in the dictionary. Because of the stable yet flexible design of CIF, the large archive of CIFs built up over the last decade will be able to exploit this feature, allowing the user to retrieve derived information that may not be explicitly stored in the CIF.

The session described a field expanding so rapidly that, even though software and dictionary developments may have difficulty keeping up with each other, the CIF project remains on the cutting edge of information technology and the opportunities for developing innovative software have never been greater.

David Brown

MEETING REPORT

X-ray structure school



The second school on X-ray structural analyses '*Analyse Structurale par Diffraction des Rayons X, Structures Absolues, Macles, Incommensurables*' was held in Toulouse, France, September 23-27, 2002, chaired by J.C. Daran (CNRS ,Toulouse) and C. Lecomte (U. Henri Poincaré and CNRS, Nancy). This school was sponsored by the CNRS, the French Ministry of the U. (Physics and Chemistry grants) and the French Assn of Crystallography (AFC, Assn Française de Cristallographie). It was also funded by different manufacturers, Alexandre Lab, Bruker-Nonius, Elexience, Oxford-Diffraction and Stoe.

Various topics were covered in the school, which was divided into two parts. The first part was devoted to the fundamental theory of crystallography, data collection , data reduction, structure solution, least-squares refinements and demonstration of the Cambridge Structural Database. The second part was related to some difficult problems as absolute structure determination, modulated structures and twinning. Practical work sessions concerning the structure solution computer programs (Shelxl, Crystals, SIR, MoPro) were organised as well as hands on sessions. Most lectures and all tutorials were taught using the French language.

Lecturers and topics included Direct and Reciprocal Space (N. Ghermani, France) Crystal Symmetry (H. Flack, Switzerland), Scattering and Structure Factors (C. Lecomte, France), Data Reduction (S. Pillet, France), From Punct to two Dimensional Detectors (M. Pierrot, France), Direct Methods (C. Giacovazzo, Italy), Patterson Analysis (J.P. Legros, France), New Developments in Direct Methods (H. Gornitzka, France). Incommensurate Structures (V. Petricek, Czech Republic), Least-Squares refinements (D. Watkin, UK), Introduction to twinning (S. Parsons, UK), Absolute Structure and Absolute Configuration (H. Flack, Switzerland), Interpretation of Results (L. Ricard, France), Data Deposition, CIF (J.C. Daran, France), Cambridge Structural Database (K. Lipscomb, F. Allen, UK), Multipolar Refinement and Charge Density Analysis (C. Lecomte, France). The atmosphere was excellent, with a lot of discussions between scholars and students around coffee, beer and glasses of French wine.

There were 70 participants coming not only from France, but also from Morocco, Algeria, Tunisia, Croatia and the Ivory Coast.

Jean-Claude Daran

MEETING REPORT

Structural genomics taskforce on publication

The first meeting of the Int'l Structural Genomics Organization (ISGO), held in Berlin last October afforded the opportunity for the various taskforces working to coordinate international efforts in structural genomics to report to the wider structural biology community. The Taskforce on Publication, chaired by G. Dodson, had earlier reached the conclusion that publication of the results of structural genomics projects in peer-reviewed articles was highly desirable. This was despite the rational criticism that augmented deposition in the Protein Data Bank (PDB) would obviate the need for 'traditional' publication. The taskforce reasoned that publication added value and provided the opportunity for interpretation of the structural results including speculation on the mechanism, function and biological role of the target protein. Such publications will bring important research and professional benefits, particularly to young scientists. Rapid and easy publication of a large number of structures, expected to result from both structural genomics and other high throughput projects, will require the type of close liaison with the PDB that currently exists between the small molecule crystallography community and the Cambridge Structural Database. In the case of proteins, however, deposition of the atomic parameters and the experimental amplitudes and associated phase information in the PDB will be the primary event. The PDB will require additional information from the depositor to describe the experiment fully from cloning and expression of the protein to refinement of the structure. The Editors of *Acta Crystallographica D* are currently working with the PDB to facilitate the transfer of the deposited data to the journal in a seamless, machine readable form. In addition a depositor to the PDB will receive a validation report on their structure, which they can submit with the manuscript to the journal of their choice for viewing by selected referees. This will ensure that the referees have access to information they require to validate the structure quickly and thus speed-up one of the rate limiting steps in the publication process. Several journals including *Acta Crystallographica D*, the *Journal of Structural and Functional Genomics and Proteins*, *Structure*, *Function and Genetics* have indicated that they will publish the results of structural genomics efforts and will welcome approaches from interested laboratories. Most of these journals either plan or already publish structural genomics papers electronically. There is still resistance in the wider scientific community to electronic-only publication, but the taskforce considers that it is ideally suited to rapid communication of high throughput structural biology results, software and techniques. It is fair to say that to date there has not been a flood of papers, but given the rate at which the various structural genomics projects are reaching the production phase the expected avalanche of structures and papers, will not be too far in the distance. Journal publishers, by nature a conservative group, have to formulate business plans to cope with prospective changes in demand which has yet to materialize.

J. Mitchell Guss and Guy Dodson

AWARDS AND PRIZES

First Jeffrey awards presented

Four Jeffrey Awards were presented at the Geneva IUCr Congress. These awards were made to outstanding graduate students in order to assist them in presenting their work at the Congress. The first Awards were each for \$520, sufficient to cover registration and student housing costs. The Award Committee (H. Berman, M. Caffrey and B. Craven) was unanimous in choosing the Awardees from a total of fifteen applicants. The Awardees in 2002 were:

Daniel Riley (U. of Newcastle, New South Wales) for rapid (0.9s) neutron diffraction data collection and differential thermal analysis which he used to follow a phase transition in titanium silicon carbide; **Mr. Rudresh** (Indian Inst. of Science, Bangalore) for his *de novo* design and subsequent structure determination of a hairpin eicosapeptide containing 3_{10} helices with opposite handedness; **Liliana Sampaleanu** (Hospital for Sick Children, Toronto) for her structure determination of duck delta1 and delta2 crystallin leading to a better understanding of the enzymatic mechanism of argininosuccinate lyase; and **Martin de Yonge**, (U. of Melbourne, Victoria) for his precision measurements of the X-ray mass attenuation coefficient for molybdenum using synchrotron radiation.

These awards were made from a fund established in memory of George A. Jeffrey. Contributions came from many of his colleagues and former students and from his family. The Jeffrey Fund is administered by the Pittsburgh Diffraction Society. The next Jeffrey Awards will be in time for the Florence IUCr Congress.

Bryan Craven

AWARDS AND PRIZES

Cotton medal awarded to G.A. Somorjai



Gabor A. Somorjai, Prof. of Chemistry at the U. of California, Berkeley, and a principal investigator in the Materials Sciences Div. of the Lawrence Berkeley National Lab, will receive the 2003 F. A. Cotton Medal sponsored by the American Chemical Soc., Texas A&M Section and the Texas A&M U. Chemistry Dept. Somorjai was chosen for his pioneering research on the chemistry of surfaces in ultrahigh vacuum and heterogeneous catalysis.

Susan Kegley

NOTICE

Symmetry video game



We have created a Video Game for teaching school children about symmetry. Symmetry is very important in every day life. We see it in birds, animals, buildings and in paintings in Mosques and Churches. It also occurs naturally in minerals. School children benefit from recognizing symmetry in nature, which will help them in their later studies. They discover that behind each symmetry a structure exists and related properties are found. This video presentation uses birds, buildings and designs from mosques and old buildings to illustrate mirror images and other symmetries. The video includes simple games to engage the students interest. We have distributed the Video-Game CD. L. Cranswick has agreed to include it in the NEXUS or release it on the internet along with the instructions for use.

Karimar El-Sayed

NOTICE

Congratulations...

Gautam R. Desiraju, U. of Hyderabad, India was recently elected as a Fellow of the Third World Academy of Sciences (TWAS). TWAS, with its headquarters in Trieste, is an association for the promotion of scientific excellence for sustainable development in the Third World. 43 new fellows were elected in October 2002, of which 4 were in the area of chemical sciences.

AWARDS AND PRIZES

The Carl Hermann medal



The establishment of the Carl Hermann Medal for outstanding contributions to the science of crystallography, was announced in August 1994 by the German Soc. for Crystallography (DGK). The name of the Medal was chosen to recognize Professor Hermann's (1898-1961) significant contributions to the foundations of crystallography. After his studies at Göttingen (with Max Born and Werner Heisenberg) he became a lecturer at Stuttgart, where he together with Paul P. Ewald initiated the *Strukturberichte*, the famous reference series (with its successor *Structure Reports*) of every known crystal structure determination. Moreover, he developed, with Charles Mauguin (1878-1958), a systematic nomenclature for the 230 space groups, from which the symmetry can be derived at a glance (so called Hermann-Mauguin notation). Throughout much of the Second World War he and his wife were imprisoned for helping Jews. In 1947 he was appointed to the chair of crystallography at Marburg U. where he built up an internationally recognized research school.

The award consists of a medal and a certificate of recognition. It is presented every year during the Annual Conferences of the DGK. Proposals can be put forward by members of the DGK (for details visit www.kristall.erdw.ethz.ch/DGK). The previous medals have been awarded to Gerhard Bormann, Hartmut Bärnighausen, Siegfried Haussühl, George Sheldrick, Heinz Jagodzinski, Theo Hahn and Hans Wondratschek.

Peter Paufler