LETTER FROM THE PRESIDENT

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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The IUCr Newsletter is distributed to 587 libraries and 15,000 crystallographers and other interested individuals in 39 countries. The IUCr also runs Crystallography Online, available at www.iucr.org, as a complement to the IUCr print newsletter. Feature articles, meeting announcements and reports, information on research or other items of potential interest to crystallographers should be submitted to the editor at any time. Submission of text by electronic mail and graphics, slides or photographs by express mail is requested. Items will be selected for publication on the basis of suitability, content, style, timeliness and appeal. The editor reserves the right to edit. Cost of distribution in Australia, Colombia, Croatia, Cuba, Czech Republic, France, India, Italy, Japan, Malaysia, New Zealand, Poland, Portugal, South Africa, Switzerland, Taiwan, The Netherlands, Thailand, and Venezuela is borne by crystallographic associations or institutions or by individual crystallographers in these countries. Address changes or corrections and requests to be added to the mailing list should be addressed to the editorial office. If you would like to see a copy of the IUCr Newsletter in your college or university library, send the address to the newsletter office so that we can add it to our mailing list.

William L. Duax
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Florence, Italy, August 23 - 31, 2005

Why Florence?

The international fame of Florence as an art city, the worldwide interest in its artistic heritage and its cultural traditions, its geographic position, the famous “green” region of Tuscany, Florence also has the advantage of having Congress facilities right in the middle of the city's business centre, near all the major hotels and tourist attractions and at a stone's throw from the railway station and from the airport terminal. Florence has all the necessary facilities: an airport with daily flights from the most important European capitals, an important railway junction which links Florence to Rome and Milan, a motorway which connects Florence with Siena, San Gimignano, Arezzo, Pisa and Lucca and the famous Chianti area, an efficient train connection system and motorway from Pisa airport.

Florence also hosts an important University and many renowned research centers. A major renovation of the scientific infrastructures is under development. A new big Campus (Polo Scientifico) is about to be fully operative.
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 co-editors 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

Correction:
Volume 10#3. The photo on pages 15-16 was courtesy of Caroline Duax (not W.L. Duax)

In the past, a number of crystallographers in the US and Europe who were no longer actively engaged in research have donated their collection of Acta Cryst Journals and other crystallographic books to a crystallographic association (i.e. ACA, BCA) that subsequently located a home for the journals and books in institutes where students need them. For example, at the present time crystallographers in Moldova could use back issues of Acta Cryst. If you have Crystallographic books and journals that you would like to donate to the next generation of crystallographers please use the IUCr Newsletter as a vehicle to let the community know. The IUCr Newsletter office will be happy to assist you in locating a recipient and facilitating the transport.

**Can a multipole analysis faithfully reproduce topological descriptors of a total charge density?**
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). B101, 5794–5799] extremely well.

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**An exceptionally stable peptide nanotube system with flexible pores**
Carl Henrik Görbitz

In a series of data collections on a selected single crystal of the dipeptide L-Ala-L-Val, space group P61, 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.

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**Acta Cryst. (2003). C59, m18–m20**

**Dichlorobis(l-proline-κO)zinc(II)**
Martin Lutz and Ruud Bakker

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 L-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.

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**PHENIX: building new software for automated crystallographic structure determination**

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.
IUCr Activities

Crystallography at High Pressure

Orsay, France, September 4-9, 2001

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. Irié 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, P. Urayama, and exciting recent progress in structural refinement of diamond-anvil-cell data from proteins presented by R. Fourme, P. Dera described experimental studies of H-bonding compounds, spin-ladders, intermediate valence systems, and highly unusual physical phenomena in magnetically unstable 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 discribed 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 as an amazing experimentalist and an enthusiastic conference organizer, friend and 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 continued on page 8...
IUCr Activities

Participants at the Crystallography at High Pressure - 2001 international workshop in Orsay, France.

(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$_6$0! N. Serebryanaya (poster oral) claimed that this new phase formed from C$_6$0 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$_2$RuO$_4$. 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$_6$0 phases and T. Watanuki for his poster on quasicrystals (tied for second).

Igor Goncharenko and Richard Nelmes
IUCr 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 MgB₂ and Related compounds

J. Akimitsu (Aoyama-Gakuin U., Japan) described the structure, effects of substitution and physical properties of this superconductor exhibiting the highest Tc (39K) among metal and alloys. The discovery of superconductivity in MgB₂ 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).

Elspeth Garman

The Good, The Bad and The Ugly; Experiences at the Synchrotron

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 synchrotron beamlines, and how data quality might be affected by reduced experimenter intervention.

Evgeny Antipov

Structural Mechanisms of Self-Assembly and Polymorphic Supercoiling of the Bacterial Flagellum

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

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

continued on page 14
to 4Å resolution and give only one image per crystal. So far, 2,317,561 reflections 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

**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. A58 (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?

Mitchell Guss

**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

Michael Woolfson with the Ewald Prize at the Opening Ceremony

**Contributions 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
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.

Emil F. Pai

David Brown
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, Elekience, 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, 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. Ried, 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

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 materialise.

J. Mitchell Guss and Guy Dodson
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

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

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

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.

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 Strukturbücher, 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
**Future Meetings**

**ACA 2003 Summer Courses**

Small Molecule Crystallography  
Indiana, PA, August 3 – 13

This course will be offered August 3-13, 2003 at the Indiana U. of Pennsylvania. There will be morning lectures on single crystal and powder diffraction methods, followed by afternoon and evening workshops for problem solving and crystal structure determination. Attendees are encouraged to bring single crystals or powder samples for X-ray data collection. Attendees are expected to have an undergraduate science degree. No prior X-ray experience is necessary, but attendees are advised to read “Crystal Structure Analysis: A Primer”, by J.P. Glusker and K.N. Trueblood, Oxford Univ. Press (1985).

The organizers aim for a total of 30 attendees. Tuition will be $200. Dormitory housing at IUP is available for $294. Fifteen scholarships will be offered. These will consist of a waiver of tuition and dormitory costs. The scholarships will be awarded based on the student’s (1) scientific ability, (2) expected benefits from the course and (3) skills in English. Special funds will be available to assist applicants from Latin America.

Instruments available will be two Bruker-Nonius single crystal diffractometers (a CAD4 at IUP and a modern instrument with CCD detector located at the U. of Pittsburgh - electronically linked to the X-ray Lab at IUP). Also available will be a Bruker-Nonius D8 powder diffractometer. There will be adequate computing facilities including access to the Cambridge Structural Database and the ICDD powder diffraction database.


Registration forms are available on the ACA website. Completed forms must be received before June 1, 2003. Further information will be updated on the website or can be obtained from craven@icubed.com.

The organizers of this Course acknowledge sponsorship not only by the ACA, but also the IUCr, the Pittsburgh Diffraction Soc. and Bruker AXS, Inc. We shall observe the basic policy of nondiscrimination and affirm the rights of scientists throughout the world to adhere or to associate with international scientific activity without restrictions based on nationality, race, color, age, religion, political philosophy, ethnic origin, citizenship, language, or sex, in accordance with the Statutes on the Int’l Council of Scientific Unions. At this Course, no barriers will exist which would prevent the participation of bona fide scientists.

Bryan Craven and Charles H. Lake, Organizers

**Electron Crystallography: Novel Approaches to Structure Determination of Nanosized Materials**  
Erice, Italy – June 9 –20, 2004

The third meeting of this kind at Erice, the thirty-sixth organized by the crystallographers since 1974, will be directed by T. Weirich (Aachen), J. Labar (Budapest), and X. Zou (Stockholm). Topics will cover general reviews of the background and the most recent techniques, Structure from HREM and Structure from Electron Diffraction, with a series of sessions on nanosized materials. Several practical workshops are also planned. For further information, visit www.crystalerce.org.

**APERICIOD 2003**  
Belo Horizonte, Brazil, September 8-13, 2003

APERICIOD have taken place every 3 years, since 1984, under the auspices of the IUCr. In 2003 it will be held at the U. Federal de Minas Gerais, in Belo Horizonte, Brazil, September 8-13.

The conference intends to promote the development of common methods and nomenclature for the crystallographic investigation of aperiodic systems, including modulated structures, polytypes, incommensurate misfit or composite crystals and quasi-crystals. It also seeks to promote scientific exchanges among working in the various fields of aperiodic materials. Special emphasis will be given to multidisciplinary aspects of aperiodicity.

For further information visit http://agora.grude.ufmg.br/apericodic2003.

Nivaldo L. Speziali

**IUCr Newsletter**  
Volume 10, Number 4  
2002
FUTURE MEETINGS

ACA 2003, July 26-31, 2003
Northern Kentucky Convention Center, Covington, KY

The organizers of ACA2003 invite you to attend an action-packed week of science and fun!

Covington, Kentucky is located across the Ohio River from Cincinnati, Ohio and is minutes from the Cincinnati/Northern Kentucky International Airport. All scientific sessions, posters and the exhibit show will be held in the Northern Kentucky Convention Center (www.nkycc.com/).

The ACA2003 meeting (www.che.uc.edu/aca/) agenda:

- Workshops: Saturday, July 26
- Scientific Symposia and Sessions: Sunday, July 27 - Thursday, July 31
- Poster Sessions: Sunday, July 27 - Tuesday, July 29
- Vendor Exhibits & Sponsored Activities scheduled throughout the week

Consult the Call for Papers for detailed information on workshops and sessions (www.che.uc.edu/aca/callforpap.pdf)

Social Events:
- Saturday, July 26 — Opening Reception: Newport Aquarium
- Sunday, July 27 — Mentor/Mentee Dinner: Chez Nora
- Monday, July 28 — Midweek Mixer: Jack Quinn’s Irish Pub
- Wednesday, July 30 — Banquet: Embassy Suites Hotel
- Thursday, July 31 — Riverboat Dinner Cruise

Symposia:
- Transactions Symposium: Neutron Diffraction (co-organizers: G. Bunick & L. Hanson)
- Special Symposium: Time-Resolved Crystallography (co-organizers: P. Coppens & K. Moffat)
- Martin J. Buerger Award Symposium: 2003 Awardee is James Ibers (Northwestern U.)
- Bertram Warren Award Symposium: 2003 Awardee is Takeshi Egami (U. Pennsylvania)

Oral Sessions:
- Crystallographic Computing
- Modulated Structures
- Important Science from Small-Molecule Structures
- Service Crystallography Laboratory Practices
- Structure Determination from Powder Data
- Characterization of Biological and Medical Fibers
- Protein Structure, Function & Dynamics
- Crystal Engineering, New Techniques and New Crystals
- Neutron Instrumentation Advances in Scattering & Diffraction

Important Upcoming Dates:
- Abstract deadline: March 1, 2003 (check website for possible deadline extension)
- Advanced Registration deadline: June 1, 2003
- Advanced Hotel Registration deadline: June 24, 2003

On-line registration and further meeting information will be posted to the ACA2003 site: www.che.uc.edu/aca/ or see the ACA web site: www.hwi.buffalo.edu/ACA/

Workshops:
- Crystals & Rotax Suite of Programs for Chemical Crystallography
- CCP4 Suite of Programs for Macromolecular Crystallography
- Cambridge Structural Database
- Crystallization Techniques & Secrets

Local Chair: Bobby Barnett, U. Cincinnati, barnettbl@cinci.rr.com
Program Chair: Jeanette Krause Bauer, U. Cincinnati, jeannette.krause@uc.edu
Social Chair: Ann Wolff, Procter & Gamble, wolff.am@pg.com
CRYSTALLOGRAPHIC MEETINGS CALENDAR

A selection of future meetings. Lists appear regularly in J. Applied Crystallography, the BCA Newsletter and the ACA Newsletter. Corrections and new listings are invited by the Editor.

APRIL 2003


MAY 2003


JUNE 2003


JULY 2003

7-10 ♦ AFC 2003. See page 22.


26-31 ♦ ACA Annual Meeting. See page 22.

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Advertising information is available at www.hwi.buffalo.edu/iucr/IUCr-News/iucrnewsletters.html

AUGUST 2003


24-30 ♦ 21st European Crystallographic Meeting. Durban, South Africa. (Call for Papers was published in IUCr Newsletter, Vol 10, No 3) www.ecm21-africa.co.za.

SEPTEMBER 2003


JUNE 2004


JULY 2004

17-22 ♦ ACA Annual Meeting. Chicago, IL, USA. www.hwi.buffalo.edu/ACA/.

AUGUST 2005


LETTERS TO THE EDITOR

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