

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



The Commissions of the IUCr are vital to its growth and development. Commission Chairs have the responsibility to see to it that the interests of a Commission are fully represented at the IUCr Congress, in the publication program of the Union, and at other national and international meetings and workshops. The Commission Chairs also have the responsibility to ensure the continuity of a Commission by attracting and appointing suitable members and consultants, by encouraging their cooperation and by appointing a suitable successor after their three years of service as Chair.

In order that all aspects of modern crystallography be properly addressed at the IUCr Congress in Florence in 2005, the Chair of the Program Committee, Carlo Mealli, has sought input from all Commissions on the composition of the Program Committee and the scientific program. You may want to contact members of the Commissions responsible for topics of interest to you to urge them to respond to requests from Carlo. I encourage you to lend your support to their efforts and offer your suggestions concerning suitable microsymposia topics.

Commission Chairs have also been asked for suggestions to expand and improve the publication programs of the IUCr in order to meet the needs of our changing and growing community. The Executive Committee is interested in suggestions for new volumes of the International Tables that address the needs of different segments of the crystallographic community represented by the Commissions. For example, there might be volumes of tables devoted to powder diffraction, high pressure studies, or crystal growth technology. If you have any ideas about publications to serve the needs of a Commission, please contact the appropriate Commission Chair.

A common complaint of Commission Chairs is that Commission Members are unresponsive to requests for suggestions and participation. At the same time, members of the Executive Committee hear that many countries are under-represented on IUCr Commissions. I urge crystallographers in under-represented countries to nominate suitable people for appointment as consultants on appropriate Commissions. Nominees should offer specific ideas and plans of how they would strengthen the Commission through their hard work and creativity.

When reviewing the composition of the Commissions, I was surprised to discover that ten member countries (Bulgaria, Chili, Croatia, Hungary, Korea, Mexico, New Zealand, Poland, Portugal, and Serbia) do not have a representative on any of the 14 IUCr Commissions. Other countries that are under represented on Commissions include China, Czech Republic, Finland, Israel, Norway, Spain, Slovenia, Taiwan, and Venezuela. We also need qualified consultants or potential Commission Members in countries that are not presently members of the Union. During my visit to Algeria, I was pleased to learn of activity in the areas of neutron powder diffraction, single crystal studies of organic and inorganic compounds, and charge, spin and electron density studies among crystallographers who might be suitable Commission members.

Commissions are encouraged to organize workshops and symposia in order to advance their science, bring new technology to developing countries, and educate and inform the next generation of crystallographers.

From 1997 through 2001, thirteen of the IUCr commissions endorsed applications to the IUCr Calendar Committee for support for student attendance at 26 workshops and symposia. Some Commissions organize sessions in all non-Congress years and others rarely organize a meeting. If a workshop or symposium on a Commission topic would be of benefit to crystallographers in your country, please contact the appropriate Commission Chair to discuss the procedures to be followed to plan a workshop or symposium.

Bill Duax

duax@hwi.buffalo.edu

EDITORIAL

Guest editorial - Michael G. Rossmann



The IUCr Congress met in Kyoto in the summer of 1972. The meeting schedule was largely a copy from previous congresses leaving little space for biological results. However, at that time protein crystallography was just starting on its initially slow, but ever more rapid exponential climb to the front seat of the crystallographic arena. The structures of myoglobin and hemoglobin had been determined in Cambridge in the late 50's, and those of lysozyme, ribonuclease, chymotrypsin, papain, as well as lactate, malate and alcohol dehydrogenase had been elucidated in the US, UK, the Netherlands and Sweden in the 60's or early 70's. Some common features were starting to be recognized, like the globin fold, the dinucleotide binding fold, and the catalytic triad of chymotrypsin. But there was no ready forum where these exciting events could be discussed in Kyoto (although Max Perutz and Walter Hoppe had organized memorable meetings attended by a few dozen crystallographers in the Austrian Alps).

Tom Blundell in England, I through my participation in the US National Crystallographic Committee, and especially Dorothy Hodgkin's organization of the IUCr meeting in Amsterdam in 1975, started to change the situation. Since that time there has been an ever-increasing presence of biology in the deliberations of the IUCr committees, although some changes took a little bit of extra push. Eventually biological crystallography was honored with its own journal, *Acta Crystallographica D*, outstandingly managed by Jenny Glusker since its inception in 1993. Then, in about 1994, the IUCr's executive committee decided it wanted to make sure of its role in the taming of the young cuckoo science before it became too big for its nest. Thus Ted Baker was commissioned to convince me to write a book on *Macromolecular Crystallography*, which was to be the gold standard for the subject. However, book writing is not my favorite occupation. Thus I avoided making any commitment by giving advice instead, hoping that Ted would eventually become tired of consulting with me. But Ted is a sly Kiwi and he completely outwitted me.

One day, in April 1996, just four months before the IUCr Congress in Seattle, I woke up realizing that I was expected to create a new volume of the *International Tables* explicitly about macromolecular crystallography. Some years earlier Eddy Arnold and I had written a chapter on Patterson methods for *International Tables Volume B*. Thus I felt that Eddy might be able to help me out of my predicament, and indeed that is exactly what happened. We had many long phone conversations in which we worked out the chapters that would be needed to give as complete as possible coverage of the now vast subject. At Eddy's urging, we expanded the initial purely crystallographic outline to review the current status of structural biology. By the Seattle IUCr meeting we already had contacted many potential authors with whom we discussed our ideas. Five years later, in 2001, we were proud to see the completion of the work, having received outstanding and full support by more than 100 authors who contributed to volume F. Eddy and I feel honored to have been editors of this volume and thank all the very many people who participated. We would now like to see volume F and some of the other volumes made available on-line. It is much more convenient to plug in my little lap-top computer most any place on Earth (I have even done so in Antarctica) than to carry around many pounds of wood pulp.

I would not believe it possible to see so much change in crystallography since I helped Max Perutz to determine the structure of hemoglobin (and since that meeting in Kyoto) had I not actually been a witness to these events. Although nothing just like this will ever happen again, I suspect that some of the most exciting discoveries are always happening right now.

Michael G. Rossmann

LETTER TO THE EDITOR

Diffractometer request

Dear Judy,

We are a crystallographic group from the Physics Inst. of the Federal U. of Goiás (www.fis.ufg.br) engaged in small molecules structural determination since 1982. In order to improve our research facilities, we ask for someone that could help us through the contribution of one diffractometer similar to CAD4 (kappa geometry). Please contact lariucci@fis.ufg.br.

Ivo Vencato and Carlito Lariucci

LETTER TO THE EDITOR

Date error

Dear Editor,

I read the IUCr news letter regularly. It is quite good in the get up and in contents. The latest issue outer cover gives Vol. 10, Number 3, 2002, but inside pages Vol. 10, Number 3, 2003. I would like to know which one is correct. This may be printers devil, which can be avoided in future.

Subramanian Natarajan

Dear Subramanian,

The inside pages should have read Vol. 10, Number 3, 2002.

Judy

LETTER TO THE EDITOR

Well done

Please let Judith know that she and all of you are doing a wonderful job with the IUCr Newsletter. I know that Bill is difficult to emulate, but all of you are doing a great job there

Hector Novoa de Armas

LETTER TO THE EDITOR

Known structure

Dear Editor

In the latest *IUCr Newsletter* (vol. 11. No 1, p.7) you reported on the article in *Acta Cryst*, E59 (2003) describing the structure of trichloroacetic acid.

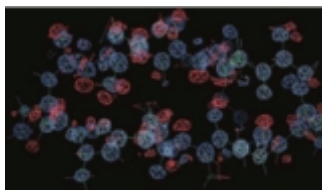
Maybe it is worth noting that neutron diffraction structure of this crystal has been known since 1972 at least (P.-G. Jonsson, W. C. Hamilton, *J. Chem. Phys.*, 56, 4433 (1972)).

T. Lis and K. Slepokura

IUCR JOURNALS NEWS

The phase problem in neutron crystallography

***Acta Cryst.* (2003). A59, 250-254**



Initial E map of the cyclosporin structure solved by *Neutron Shake-and-Bake*. The initial r.m.s. phase error is 37° . The hydrogen sites are displayed in negative (red) density while the C, N, O skeleton is displayed in positive (blue) density.

The crystallographic phase problem is formulated as a problem in constrained global minimization. In contrast to traditional direct-methods techniques using X-ray diffraction, this formulation does not require that the density function be positive everywhere. Instead, suitable generalization of the well known *Shake-and-Bake* formalism, here called *Neutron Shake-and-Bake*, exploits prior knowledge that the density function, as called for in the neutron diffraction case, is now permitted to assume negative, as well as positive, values. The initial application is made to the solution by *Neutron Shake-and-Bake* of the 199 atom (113 hydrogen atoms plus 86 nonhydrogen atoms) cyclosporin structure using experimental neutron diffraction data alone. Comparing the relative ease of this structure determination with the far greater challenge posed by the deuterated cyclosporin isomorph, in which the density function is positive everywhere, shows that, in sharp contrast to the prevailing view, the positivity of the density function not only does not facilitate, but actually substantially hinders, the phase determination process.

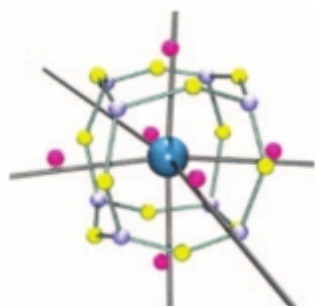
H. A. Hauptman and D. A. Langs

IUCR JOURNALS NEWS

Experimental charge density in the transition metal complex $\text{Mn}_2(\text{CO})_{10}$: a comparative study

Experimental charge density in the transition metal complex $\text{Mn}_2(\text{CO})_{10}$: a comparative study

Acta Cryst. (2003). B59, 234-247



For compounds of the transition metals, a simplistic topological analysis based solely on the density $\rho(\mathbf{r})$ and the Laplacian of the density $\nabla^2\rho(\mathbf{r}_b)$ at the bond critical points (bcp) is misleading. Our study on $\text{Mn}_2(\text{CO})_{10}$ concurs with previous work and shows little detectable charge build up between the Mn atoms. However, a significant direct Mn-Mn interaction is indicated by the (small) negative value of total energy density $H(\mathbf{r}_b)$ at the bcp and the integrated density over the interatomic surface. There is excellent agreement between the experimental density and that derived from DFT calculations at the 6-311+G* B3LYP level.

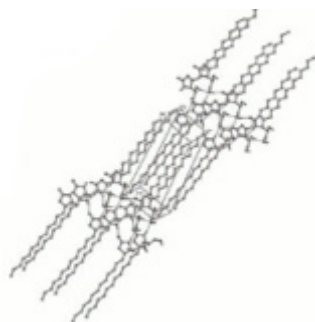
Louis J. Farrugia, Paul Mallinson and Brian Stewart

IUCR JOURNALS NEWS

(4*S*,5*S*)-4-[(1*R*)-1,2-Dihydroxyethyl]-5-tridecyl-1,3-oxazolidin-2-one

(4*S*,5*S*)-4-[(1*R*)-1,2-Dihydroxyethyl]-5-tridecyl-1,3-oxazolidin-2-one

Acta Cryst. (2003). C59, o225-o227



Amphiphilic lipids are composed of a polar head group and an apolar tail of one or two hydrocarbon chains. Depending on the space requirement of both building blocks, they form micellar (one alkyl chain) or lamellar (two alkyl chains) structures in the aqueous environment of living systems.

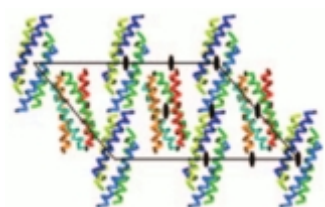
In the crystal, a 1,3-oxazolidin-2-one substituted with a polar dihydroxyethyl and only one tridecyl residue forms alternating layers of hydrocarbon chains and polar head groups. The molecules arrange in intercalating bilayers with a lipophilic core and a polar surface, in which the head groups are connected within and also between the layers by a network of hydrogen bonds.

Peter Sawatzki, Thomas Mikeska, Martin Nieger, Michael Bolte and Thomas Kolter

IUCR JOURNALS NEWS

Structure determination of a small protein through a 23-dimensional molecular-replacement search

***Acta Cryst.* (2003). D59, 709-718**

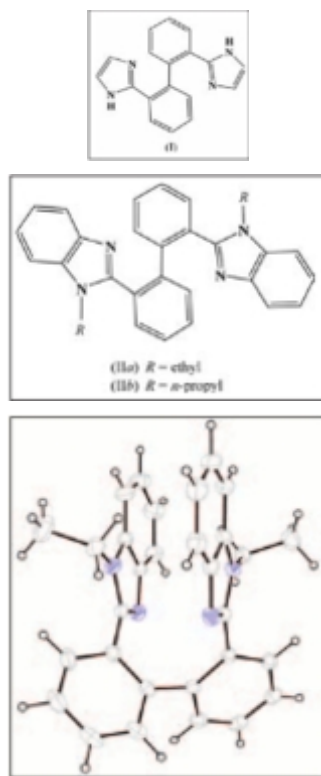


We have recently described a multidimensional molecular-replacement method that attempts to simultaneously and independently determine the positional and orientational parameters of all molecules present in the asymmetric unit of a target crystal structure through a reverse Monte Carlo optimisation of a suitable statistic (like the *R* factor or the linear correlation coefficient between the observed and calculated structure factor amplitudes). This paper reports the successful application of this method to a 23-dimensional molecular-replacement problem, allowing the determination of the crystal structure of a 4- α -helical bundle protein. The search model for the calculation was a 26-residue-long polyalanine helix amounting to less than 13% of the total number of atoms in the asymmetric unit of the target crystal structure.

N. M. Glykos and M. Kokkinidis

2,2'-Bis(1-ethylbenzimidazol-2-yl)biphenyl

Acta Cryst. (2003). E59, o693-o695

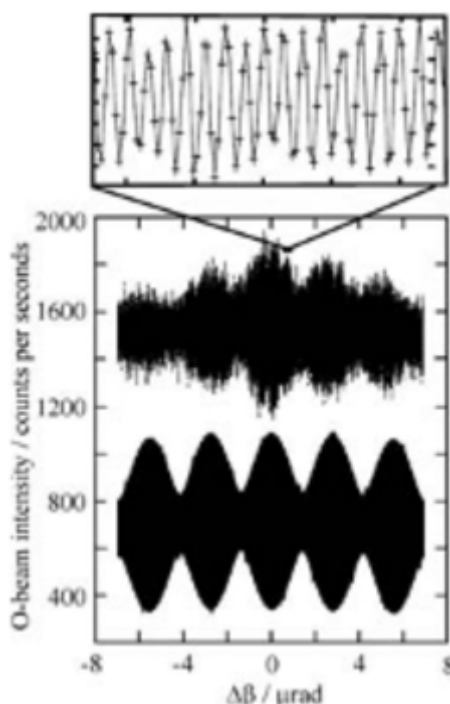


Biphenyl-linked bis(imidazoles) (I) and bis(benzimidazoles) (II) act as flexible, geometrically constraining bidentate ligands containing four planar groups and three torsional degrees of freedom. They have been used in studies of electron self-exchange, to enforce near-tetrahedral coordination in transition metal complexes, in catalysis, and as proton sponges. In the solid state, II, *R* = ethyl adopts an unusual, compact, twisted-clamshell conformation with site symmetry 2 (ethyl groups *trans*). The shortest distances between C and N atoms of the *nearly eclipsed*, slightly diverging imidazole fragments range from 3.167(3) Å to 3.673(3) Å, indicative of strong intramolecular π - π interactions. In contrast, II, *R* = *n*-propyl exhibits an open structure with little evidence of intra- or intermolecular π - π interactions.

Robert T. Stibrany, Harvey J. Schugar and Joseph A. Potenza

A Michelson interferometer for X-rays capable of high-order measurement

J. Appl. Cryst. (2003). **36**, 269-279



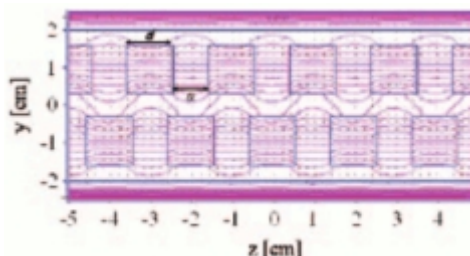
Top: Scan of 18 single orders. Middle: Measured Fourier spectrum over a total of 1704 orders of the copper $K\alpha_1$ - $K\alpha_2$ doublet. 4 beat nodes are recognizable. Bottom: Calculated Fourier spectrum of the same order range.

The first Michelson interferometer for hard X-rays [A. Appel and U. Bonse (1991). *Phys. Rev. Lett.* **64**, 1673-1676] featured geometric path-length differences of interfering beams of about 120 nm corresponding to 750 orders at wavelength $\lambda \approx 0.15$ nm. Using the same design principle, i.e. mixing of Laue- and Bragg-case beams diffracted by only one set of Bragg planes of two separate structures of perfect silicon crystals, the scan range could be extended by a factor of 3.6 by modifying the beam-path geometry. 2700 interference orders of the copper $K\alpha_1$ - $K\alpha_2$ doublet, corresponding to six beat nodes of the doublet, were recorded in Fourier spectrometric mode as shown in the diagram. Based on the know-how gained in this study, an extension to 40000 orders, equivalent to a spectroscopic resolution $\lambda/\Delta\lambda \approx 20000$, appears feasible.

Michael Nusshardt and Ulrich Bonse

Variable-period undulators as synchrotron radiation sources

J. Synchrotron Rad. (2003). **10**, 205-213



Basic concept for a variable-period undulator. The spaces with width α permit period variation along the z axis, and the blocks of high permeability material have a fixed width d . The periodic transverse undulator field is derived by the staggered arrays from the longitudinal field produced by a normal conducting or a superconducting solenoid.

Permanent-magnet undulators have served well in the production of bright X-ray beams. However, their fixed magnetic period limits their broad application, primarily their tunability. A novel concept for undulators with the capability to vary the length of the magnetic period for the production of synchrotron radiation is proposed based on staggered arrays of poles placed in a magnetic solenoid. The impact of such a 'variable-period undulator' on synchrotron science is very broad due its wide energy tunability and delivery of highly brilliant radiation without the burden of handling the high power load on first optics. This development would further contribute to future linac-based sources such as energy recovery linacs and free-electron lasers.

G. K. Shenoy, J. W. Lewellen, D. Shu and N. A. Vinokurov

MEETING REPORT

IUCr XIX Congress

Reports continued from Volume 11 #1



Extremes of Pressure and Temperature

This High-Pressure Commission microsymposium highlighted structural studies of materials subjected to a broad range of thermodynamic conditions up to megabar pressures and thousands of degrees. T. S. Duffy (Princeton U., USA) presented an overview of recently developed radial X-ray diffraction studies of deep Earth materials using diamond-anvil cells. These studies demonstrate for the first time that detailed information about elasticity and strength of abundant lower mantle materials can be obtained directly from measurements at the pressures of the deep Earth. S. Ono (Japan Marine Science & Technology Center) discussed high P-T X-ray diffraction studies of phase transitions of on the complex mineral assemblages peridotite and basalt. C. S. Yoo (Livermore Nat'l Lab, USA) focused on the extraordinary pressure-induced transformations of simple molecular systems such as CO₂ at high pressure, including the formation of novel framework and ionic solids. J. H. Eggert (Livermore Nat'l Lab, USA) presented new results on the transformations of water under pressure that included both X-ray measurements of structural changes and laser shock studies of pre-compressed samples that access very high temperature states at higher pressures. G. Galli (Livermore Nat. Lab, USA) offered an overview of state-of-the-art first-principles simulations of fluids at high pressures and temperatures.

Complementing the experimental talks, she presented new calculations for H_2 , H_2O , and other systems and highlighted the role of theory in uncovering new phenomena in these 'simple' systems under extreme conditions.

Russ Hemley

Protein-Protein and Protein-Nucleic acid Interactions

Microsymposium topics included three-dimensional structural views of mismatched base pair recognition by MutS, the M7GpppG recognition by the human nuclear cap-binding complex, ssDNA recognition by Replication Protein A, the Holliday junction binding by RuvA-RuvB complex and DNA recognition by a transcriptional regulator complex related to myeloid gene activation.

Kosuke Morikawa

Signal Transduction

This session highlighted the role of signaling domains and their complexes with lipids, peptides, and proteins. The multifunctionality of signaling domains involved in cell-adhesion was illustrated by two talks. T. Hakoshima (Nara Inst. of Science and Technology, Japan) described an impressive series of structures of the FERM domain of radixin in complex with each of its partners, including an analogue of the PIP2 phosphoinositide, peptides derived from the Na^+/H^+ ion exchanger regulatory protein (NHERP) and from the adhesion protein ICAM-2, and the GDI regulator of the small G protein Rho. All partners bind to independent sites with little or no overlap, providing insights into the role of this domain in coordinating signal transduction at the plasma membrane to cytoskeleton reorganization. In contrast, structures of the FAT domain, a domain that recruits Focal Adhesion Kinase (FAK) to sites of integrin signaling, which was presented by S. Arold (Centre de Biochimie Structurale, France), revealed that tyrosine phosphorylation of this domain, which triggers downstream signaling through recruitment of the SH2 domain of GRB2, is not compatible with the binding of the LD motif of paxillin, suggesting that the latter interactions must be disrupted for the signaling cascade to proceed. Moreover, phosphorylation appears to require structural rearrangements whose nature is suggested by the flexibility of the unbound FAT domain in different crystal structures. The presentation by K. Scheffzek (EMBL, Germany) provided still another picture of multifunctionality with the structure of full-length HPr kinase/phosphorylase. This enzyme regulates carbon metabolism in Gram-positive bacteria by catalyzing both the phosphorylation and dephosphorylation of HPr, a protein of the phosphotransferase system. Both activities take place at the same active site but they use different mechanisms. Observation of phosphates bound at the catalytic site and the comparison with other kinases provides hints at the catalytic mechanisms. F. Dyda (NIH, USA) described a spectacular structure of a 14-3-3 protein complexed with the full-length phosphorylated enzyme AANAT, and showed that not only does the 14-3-3 domain target the enzyme, but it instigates allosteric changes in it as well. Finally, in an interesting departure from her abstract, H. Wu (Cornell Medical School, USA) spoke about the structure of the apoptosis inhibitor p35 in complex with human caspase-8. The caspase is inhibited in the active site via a covalent thioester linkage to p35, which undergoes a dramatic conformational change upon cleavage. The repositioning of the N-terminus of p35 into the active site of the caspase blocks the catalytic dyad and protects the thioester intermediate.

J. Hurley and J. Cherfils

Plenary lecture by Joseph Schlessinger

J. Schlessinger (Yale School of Medicine, USA) presented a lecture on the mechanism of activation of growth factor receptors, an area to which he has been one of the world's leading contributors in biochemistry, cell biology, and structural biology. His focus was on the mechanism of dimerization of one such receptor, the fibroblast growth factor (FGF) receptor. The interplay between the polyanionic

sulfonated sugar heparin, FGF, and the FGF receptor was beautifully illustrated in a series of structures solved in different conformations and oligomeric states. The presentation was made with much flair and kept the audience awake throughout, but the most entertaining moment came with a video clip showing a duel between two sumo wrestlers as a metaphor for the engagement of two FGF receptor monomers. The crystallographic aspects of the study were done in collaboration with Hubbard and Mohammadi (both at NYU, USA), who were generously acknowledged. The final part of the talk gave a vignette of some of the biological aspects of growth factor receptor signaling, with a focus on a new adaptor protein in FGF receptor signaling, FRS2.

J. Hurley

High-Pressure Open Commission Meeting

High Pressure Biology and Soft Matter Under Pressure

Recently, the combination of diamond anvil cell, ultra-short wavelength X-rays from undulators and large imaging plates has allowed the extension of the field of high-pressure macromolecular crystallography both for accessible pressure range (beyond 2 kbar) and data quality. R. Kahn (IBS, France) presented measurements on hen egg-white lysozyme crystals at pressures up to 7 kbar and on cowpea mosaic virus (CPMV) which is the first example of a crystallized macromolecular assembly studied at high pressure. The possibility of obtaining accurate structural information under high pressure opens a wealth of possibilities such as exploration of sub-states, study of interactions between molecules and between subunits, and detection of the onset of pressure-induced denaturation. Furthermore, high pressure might become a standard tool to improve order in macromolecular crystals, either by favoring more ordered packing or by restricting amplitudes of atomic motions in regions which are disordered at atmospheric pressure. W. Doster (TU Munich, Germany) described dynamic neutron scattering experiments recording structural motions across the unfolding transition of myoglobin in solution. Using isotopic exchange this technique allows one to discriminate between structural fluctuations and those of the hydration shell upon pressure-induced unfolding. The effect of pressure and water penetration on the kinetics of ligand binding were discussed. J. Seddon (Imperial College, UK) described X-ray studies on the effects of pressure on lyotropic liquid crystals made of lipids. These are some of the most pressure sensitive condensed matter systems known and exhibit large changes in phase structure with changes of only a few hundred atmospheres of pressure. Seddon *et al.* found that pressure can induce the appearance of inverse bicontinuous cubic phases, which do not occur at atmospheric pressure. In addition, a pressure-jump apparatus with synchrotron diffraction was used to study the time course of transitions involving inverse cubic phases, with a view to unravelling the underlying transition mechanisms, e.g. between different bicontinuous cubic phases, and between cubic and inverse hexagonal or lamellar phases. The kinetics is found to depend on the difference between the final pressure and the pressure at the phase transition boundary. Evidence for intermediate structures occurring during the transitions was observed in several cases.

The OCM clearly demonstrated that pressure work on biomolecular and other soft condensed matter systems can yield a wealth of enlightening new information on their structure, energetics, phase behaviour and on their transition kinetics, and might promise fulfillment of the challenge set forth by W. Kauzmann when discussing thermodynamics of unfolding of proteins: 'Until more searching is done in the darkness of high-pressure studies, our understanding of the hydrophobic effect must be considered incomplete'.

Roland Winter

MEETING REPORT

XD program international workshop



A new release of the XD program for X-ray Charge Density Analysis was the immediate reason for an international workshop at the State U. of New York at Buffalo held May 12-17, 2003. Sponsorship came from the IUCr, Bruker-AXS, the Center for Computational Research and the Office of the Vice President for Research at the U. at Buffalo. Because of the emphasis on 'hands-on' instruction, the workshop was limited to 40 participants, and was fully subscribed. The new release includes integration of physical properties over topologically defined atomic basins, improved visualization, and the new relativistic wave functions for atoms and ions for analysis of compounds containing relatively heavy elements. The instructional sessions were divided into two parallel tracks. The first was to initiate those new in the field of accurate X-ray diffraction in the main methodologies of X-ray Charge Density Analysis, ranging from multipolar modeling to the application of the Quantum Theory of Atoms in Molecules. The second was to train more experienced scientists in the use of the new release of the XD programming package. P. Macchi of the Inorganic Structural Chemistry Dept. of the U. degli Studi di Milano headed the Program Committee, while A. Volkov of the U. at Buffalo made major contributions to the tutorial exercises. I. Novozhilova, also of UB, took expert care of the organization of the meeting and its social aspects, including the Niagara Falls excursion for which the sun unexpectedly appeared. Participants were unanimous in their praise for the program and the organization of the workshop, which may be repeated in two or three years on a different continent.

Philip Coppens

MEETING REPORT

Small molecules workshop

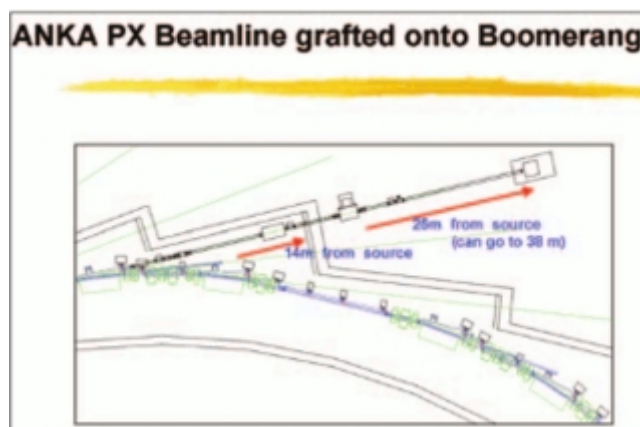


Image courtesy of Alan Jackson.

A workshop for potential users of the Australian Synchrotron was held at the U. of Melbourne School of Law, January 29-31, 2003. The workshop was part of the process of developing the first group of Australian Synchrotron beamlines to meet the needs of Australian science and industry. It brought together researchers who are using synchrotrons now and also those who could use the Australian Synchrotron in the future. International experts in synchrotron design, operation and experimentation helped enhance Australian understanding of what we can expect from the Australian Synchrotron and its beamlines.

Small molecule single crystal diffraction (SMX) made its first appearance at the workshop proceedings on the morning of the first day when R. Garret mentioned the ASRP's SCrAPS program in an overview of Australian Synchrotron research. S. Hall gave a photon fast introduction to the usefulness of synchrotron light for small molecule single crystal studies, being restricted to a maximum presentation time of 5 minutes. The new version of the Australian Synchrotron, Boomerang20, is to be bigger, brighter and better and the beamline presenters clearly had to be correspondingly faster.

In the afternoon of the second day of the workshop, participants dispersed into beamline specific discussion groups (breakout groups) to discuss and prepare detailed summaries of the needs and costs for their proposed beamlines. The small molecule demand for beam time is unlikely to require a dedicated end station in the foreseeable future. Consequently the small molecule group, represented and led by S. Hall, have primarily pursued a share in one of the two beamlines being proposed for protein crystallography (PX). Small molecule crystallography and protein crystallography have significant areas of technical and scientific overlap; more so than with any other beamline group. Accordingly, the small molecule group primarily participated in the protein breakout session. The discussion session canvassed a number of technical, managerial and financial matters, and concluded that there were good reasons and no significant obstacles in having SMX share the proposed PX micro-crystallography undulator beamline.

The SMX group was fortunate to have S. Teat (Senior Station Scientist, Daresbury Lab Synchrotron, UK) present at the workshop. Simon is the manager of station 9.8, which is currently the only dedicated small molecule single crystal crystallography station at any synchrotron. Over the past year Simon and D. Cookson, Deputy Project Manager and beamline scientist at ChemMatCARS, have provided significant and valuable information for the case for a SMX facility at the Australian Synchrotron. As a visiting researcher he has an ongoing involvement in the commissioning of the small molecule beamline at ALS. At the protein crystallography discussion group he gave an impromptu overview of the benefits of synchrotron light for small molecule crystallography, and answered questions arising from that overview. He contributed to the technical, beamline cost assessment and synchrotron management discussions of

the protein group. Simon also participated in the powder diffraction discussion group, where he gave a presentation on current trends in small molecule single crystal synchrotron crystallography.

The relevance of single crystal studies to powder diffraction was highlighted with an example of an incommensurate structure requiring single crystal synchrotron data for its structural resolution. In addition to providing structures and charge density distributions from weakly diffracting crystals, wavelength tuneable synchrotron light offers the possibility of utilising anomalous dispersion effects in single crystal diffraction, to reliably determine mixed metal site and multiple oxidation state occupancies. Simon's presentation to the powder group was followed by a brief assessment of the likely demand for SMX studies at Boomerang, from the perspective of my involvement in the SCrAPS program, and then S. Batten (Monash) further outlined areas of overlap between powder and single crystal interests from the small molecule perspective. The organisers should be congratulated for bringing potential users and experts together to more clearly define Boomerangs future shape.

Peter Turner, Scanz Newsletter No 54, February 03

MEETING REPORT

1st annual Biomaterials Workshop

1st annual Biomaterials Workshop



The Biomaterials Workshop was hosted by Cranfield U. (Shrivenham, UK) on March 17, 2003. It was the inaugural launch of a series of such meetings designed particularly to introduce new researchers to more established workers in the field and present new and emerging areas. The meeting attracted more than 80 delegates from as far away Spain and Belgium.

P. Marquis (U. of Birmingham) described conventional and new material systems for use as dental restorative materials. He convinced everyone that finding alternatives to metallic amalgams is a high technology challenge and described the potential benefits of newly developed nano-particulates as they can provide the material quality and aesthetics required. A. Lloyd (U. of Brighton), presented a method for enhancing osteointegration through exploitation of part of the natural mineralisation process, describing the role of calcium-binding phospholipids within matrix vesicles and Prof. Lloyd showed how such lipids can, *in vitro*, self assemble into 3-D gels that may provide a suitable environment for rapid calcification.

Different fabrication routes to produce apatite coatings were discussed by D. Grant (U. of Nottingham). Coatings formed by plasma spraying and laser ablation were compared with respect to their chemistry, surface topography and cell interaction. He emphasized the need to apply absorption corrections in diffraction measurements of crystallinity and pointed out the lack of any ASTM methodology in this respect. J. Knowles described the use of phosphate based glasses as biomaterials, and explained how the solubility of such materials can be significantly modified through the addition of Na or Ca ions. These glasses are relatively soluble in contrast to the bioglasses traditionally employed as biomaterials. He went on to show that, by annealing the glasses to crystallization, the subsequent phase mix can be employed to determine the amorphous structure. One use of such glasses is as 3-D fibre network structures to support cell growth systems. P. Wilshaw (U. of Oxford) described a novel approach to formation of a strongly adherent bioactive coating based upon a nanoporous alumina ceramic. The advantage of this technology is that pore diameter can be easily controlled and that these pores are typically $\sim 0.2\mu\text{m}$, which is significantly lower than conventional porous materials used for biomaterial applications. Very low dissolution rates in culture media & osteoblasts were reported (0.03% in 10 days) and the rate of Al release is also apparently very small. Cell interaction with these surfaces was illustrated and the potential for loading the pores with bioactive materials discussed.

Following lunch, delegates were able to 'mix and match' between three parallel sessions. from *an industry perspective of plasma sprayed coatings* (R. Scott, Biomet-Merck) to *bone fragility & its causes* (P. Zioupos, Cranfield U.) and *an introduction to the medical devices Faraday partnership* (F. Smith, MDPF).

J. Franks (Brunel U.) described a room temperature fabrication route for the formation of diamond like carbon coatings with high substrate adherence. These were described as being hard and flexible and good for preventing thrombus formation. Finally, J. Elliott (Queen Mary), who has been described as one of the most notable pioneers in apatite structural chemistry, carefully described the key ionic packing arrangement of the apatite lattice and pointed out that most of the space is occupied by phosphate ions packed into a pseudo-HCP arrangement. He illustrated several ionic substitution possibilities and, in

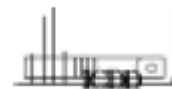
particular, carbonate substitution into phosphate and hydroxyl sites. He finished by indicating that apatites can still produce surprising results and described how his recent work has shown evidence of formate substitutions.

Further details of the next workshop will be announced in due course at www.cranfield-biomaterials.com.

K.D. Rogers

NOTICE

ICDD and MPDS collaboration



The Int'l Centre for Diffraction Data (ICDD) is pleased to announce a collaborative agreement between the ICDD and Material Phases Data Systems (MPDS), headquartered in Vitznau, Switzerland. The ICDD is a scientific organization founded by and dedicated to scientists working in the field of X-ray analysis. MPDS is focused on inorganic materials and design systems.

The collaborative agreement will result in the incorporation of inorganic structural data (S-entry) from the LPF into the PDF-4 relational database format of the Powder Diffraction File (PDF). The structural data includes atomic coordinates, crystallographic and bibliographic data. The inclusion of this data combined with ICDD's on-the-fly digital calculation technology and relational database format will enable the ICDD to deliver on its stated longterm objective of supporting total pattern analysis. With integrated software available from ICDD's licensed software developers, PDF-4 database users will be able to identify unknown materials and then quantitate the components by either the Reference Intensity Ratio (RIR) method or Rietveld methods. Identification and RIR quantitation is possible with today's integrated database; the addition of atomic parameters into the PDF will enable the Rietveld calculations. Including select LPF data will add new materials to the PDF database as well as provide complimentary atomic, crystallographic and bibliographic data to existing material sets.

Today's PDF contains 272,931 published material data sets including 34 million d-spacings and 530,000 literature citations from 1,602 journal sources. The database is made possible through the collaborative efforts between the ICDD and the Cambridge Crystallographic Database Corp. (CCDC), Fachinformationzentrum Karlsruhe (FIZ) and the Nat'l Institutes of Standards and Technology (NIST). All data sets are converted into a common format and extensively edited and reviewed by both the editors of the originating organization and again by the ICDD editorial staff. The collaboration with MPDS ensures that the PDF will have comprehensive coverage of materials characterized by X-ray analysis. As a result of continuous editing and compilation from all sources, the ICDD estimates that the PDF will grow by ~30,000 material data sets per year with over 70,000 additions this year.

AWARDS AND PRIZES

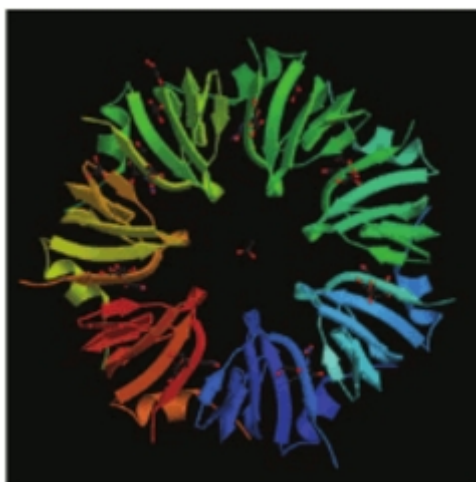
PDC news and call for nominations for the Sidhu award



The Pittsburgh Diffraction Soc. is pleased to announce that its next conference will be held in New Brunswick, NJ, at the Rutgers U. Inn, October 30 - November 1, 2003. The symposia are 'Macromolecular Complexes of Biological Interest', 'The Single Crystal - Powder Diffraction Interface' and 'Teaching Diffraction to Undergraduates'. There will be a reception and poster session on October 30 and a banquet and award ceremony on October 31, during which the Sidhu Award will be made. Nominations are herein requested for this award, which is made in honor of Professor Surhain Sidhu, to a scientist within 5 years of the PhD who has made an outstanding contribution to crystallography or diffraction. For further information and to submit nominations, please email (emge@rutchem.rutgers.edu) or mail to: T.J. Emge, Dept. of Chemistry and Chemical Biology, Rutgers, The State U. of New Jersey, 610 Taylor Road, Piscataway, NJ 08854.

NOTICE

Structure factor file check: have you deposited?



Structure factors are available for PDB entry 1lnx (Mura, C., Kozhukhovskiy, A., Gingery, M., Phillips, M., Eisenberg, D.: The Oligomerization and Ligand-Binding Properties of Sm-Like Archaeal Proteins (Smaps) *Protein Sci.* 12 pp. 832 (2003))

For many years, the Protein Data Bank (PDB) has encouraged the deposition of all experimental data by making it as easy as possible. When depositing coordinates, structure factor data can be submitted in ANY format with an accompanying description of content.

In spite of these efforts, structure factor files are available for only about half of the more than 17700 crystal structures available in the PDB (www.pdb.org).

A campaign has been started by G. Kleywegt and A. Jones (U. of Uppsala) to encourage crystallographers to deposit their structure factor data to the PDB (www.rcsb.org/pd/lists/pdb-l/200305/000743.html). A very simple query form called 'SOS - Save Our Structure factors' is available at fsrv1.bmc.uu.se/eds/eds_sos.html. Type in your name to retrieve a list of your entries that do not have structure factor data available. Once you get the list e-mail the missing structure factor data to deposit@rcsb.rutgers.edu.

The value of the PDB will be substantially increased by having a complete archive of the coordinates AND the structure factors.

Christine Zardecki

NOTICE

Update from the CCDC



Currently, the Cambridge Structural Database (CSD) contains over 290,000 structures, including the February and April data updates, available to subscribers via the Web, and a target of 300,000 structures will be close by the time of next full CSD System release in November 2003. As the number of CIFs deposited with the CCDC continues to rise exponentially, it is appropriate that April saw the release of the long-awaited CIF editor: *enCIFer* (version 1.0) from the CCDC. *enCIFer* is available for free download for *bona fide* research purposes from: www.ccdc.cam.ac.uk/prods/encifer/index.html.

The CIF (Crystallographic Information File) is now the standard means of information exchange in crystallography. An increasing number of journals require CIF depositions to be associated with new papers, and some generate papers for publication directly from CIFs. It is also the (much) preferred way of submitting data to the CSD. Being text files, CIFs can be manually edited or amended, and if this is not done correctly, programs designed to read and interpret CIF data will encounter problems. It is for this reason that *enCIFer* has been written.

enCIFer provides an intuitive interface which, having finished a crystal structure refinement, allows you to add information, e.g. bibliographic data, crystal properties, etc., safely to the resultant CIF without corrupting the strict syntax, giving rise to a format compliant file. Additionally, *enCIFer* has been designed to suit expert and novice CIF editors alike. Feedback from beta-testers has been encouraging, so please try it in your laboratory and let us know what you think (support@ccdc.cam.ac.uk).

Single and multi-block CIFs can be edited using *enCIFer* permitting:

- Location and reporting of syntax/format violations using the current CIF dictionary
- Correction of these syntax/format violations
- Editing of existing individual data items or looped data items
- Addition of new individual data items or looped data items
- Addition of certain standard additional information via two data entry wizards: Publication wizard – basic bibliographic information required by most journals and databases that accept CIF deposition files; Data wizard – chemical, physical and crystallographic property information that enhances a CIF for journal or database deposition
- 3D visualisation of structure(s) in a CIF

Many journals have arrangements whereby the CIF is deposited with the CCDC before the paper is submitted for publication. The CCDC also accepts Private Communications for structures for which formal journal publication is not envisaged. Full details about both data deposition schemes can be found on the CCDC website: www.ccdc.cam.ac.uk/conts/depositing.h

Karen Lipscomb and Susan Robertson from ACA Newsletter, Summer 2003

AWARDS AND PRIZES

ECA prize 2003



The European Crystallographic Assn is to award the third European Crystallography Prize to Carmelo Giacovazzo of the U. of Bari, Italy. Prof. Giacovazzo is being recognized for his major theoretical and practical contributions to the solution of the phase problem in a wide spectrum of applications.

The Prize will be presented during the Opening Ceremony of the upcoming 21st European Crystallographic Meeting to be held in Durban, South Africa, August 24-29, at which Prof. Giacovazzo will describe the work for which he is being honoured.

His main theoretical contributions are the Representation Theory and several probabilistic formulae for the estimate of structure invariants and seminvariants. From the practical point of view, he has directed and coordinated a research group for the implementation of widely used computer programs for the solution of crystal structures not only from single crystal data but also from powder diffraction data. More recently he has developed new and powerful methods for solving *ab-initio* macromolecular structures using data collected at atomic resolution. He has also provided a new probabilistic approach for the location of the heavy or anomalous scatterers in SIR-MIR-SAD-MAD techniques and for the subsequent phase estimation.

ECA elections

Councillors representative of the Individual Members for 2003-2006:

Giovanni Ferraris, Hans Grimmer, Paola Spadon, Elspeth F. Garman, Carlo Mealli

AWARDS AND PRIZES

ASRP Research Fellowships

The Federal Minister for Science, Peter McGauran, recently announced recipients of the Australian Synchrotron Research Program (ASRP) Research Fellowships

Barbara Etschmann, CSIRO (formerly at the South Australian Museum). Her project is: Nuclear microprobe and synchrotron-based spectroscopy of inorganic materials and solutions, opening new opportunities in fields such as hydrothermal ore processing and mineral exploration.

Joshua McKinnon, U. of New England. Optimising data collection strategies to refine synchrotron-based charge density analysis techniques.

Kia Wallwork, ANSTO (formerly at Flinders U.). Investigation of pressure-induced phase transitions using powder X-ray and neutron diffraction techniques, including the study of oxides such as zeolites.

NOTICE

50 years of DNA



From the NDB. Drew, H.R., Wing, R.M., Takano, T., Broka, C., Tanaka, S., Itakura, K., Dickerson, R.E. Structure of a B-DNA Dodecamer. Conformation and Dynamics *Proc. Nat. Acad. Sci. USA*, **78**, pp. 2179-2183, 1981.

In case you were not aware, 2003 is rather a special year in the history of crystallography as it was in the April 25, 1953 issue of *Nature*, that Watson and Crick published their famous paper on the structure of DNA (it is actually available free on the web as both HTML and also a pdf page-image of the original article: www.nature.com/genomics/human/watson-crick/). Many celebrations and events have been planned worldwide to celebrate this important work (if you don't believe me, type 'watson crick 50th dna' into Google, and see what you end up with!). Our New Zealand colleagues are even making the most of the fact that Maurice Wilkins was born there, although he returned to the UK with his parents at the age of 6, and never returned (see www.rsnz.govt.nz/news/releases/wilkins_dna.php). But as crystallographers, you owe it to yourself to go back to Volume 171 of *Nature*, and not to rely too much on the hype surrounding this anniversary. In particular, read the Watson & Crick paper (pages 737-738), and take special notice of the first sentence: 'We wish to suggest a structure for the salt of deoxyribose nucleic acid (D.N.A.). This structure has novel features which are of considerable biological interest'. Further into the brief article you will find: 'So far as we can tell, it is roughly compatible with the experimental data, but it must be regarded as unproved until it has been checked against more exact results. Some of these are given in the following communications. We were not aware of the details of the results presented there when we devised our structure, which rests mainly though not entirely on published experimental data and stereochemical arguments.'



Image by David S. Goodsell from the PDB's Molecule of the Month series.

So, you will see that the famous paper on the structure of DNA, the one that introduced the elegant double helix, is really presenting little more than a hypothetical structure. No crystallographic information is presented and no crystallography experiment was reported by Watson & Crick. So why is crystallography so inextricably connected with the discovery of the structure of DNA? The answer can be found in the 'following communications' referred to by Watson & Crick. Their article is followed immediately by a paper on the 'Molecular structure of deoxypentose nucleic acids' by Wilkins, Stokes & Wilson, and that in turn is followed by a paper on 'Molecular configuration in sodium thymonucleate' by Franklin & Gosling. Although not obvious from the titles, it is these two papers that present the crystallographic evidence, not just for a helical structure, but for the actual dimensions - radius and repeat unit - that were reported by Watson & Crick. I leave it to you to decide whether the Watson & Crick structure could have been devised while being 'not aware of the details' of the crystallographic results. In line with similar meetings worldwide, the scientific program for AsCA/Crystal23 includes a session entitled 'Nucleic Acids and Their Protein Complexes (50 Years Since the Double Helix)'.

Mark Spackman excerpted from Scantz Newsletter No 54, February 03

OBITUARY

A. T. H. Lenstra (1942 - 2002)

Albert (Ab) Lenstra died on August 18, 2002 aged 60. He was professor in structural chemistry at the U. of Antwerp (UIA). He obtained his doctorate in Utrecht, in the crystallography laboratory founded by J.M. Bijvoet. His research was in the field of X-ray structure analysis of small molecules, in particular the study of deformation densities for which he needed to give special attention to quality control of diffraction intensity measurements. Through this work he became an expert in the use of Bayesian statistics and, with his coworkers, had several publications on this domain, the last of which appeared in 2001.

Through his research, his students and his post-docs from Russia and China, Ab had many friends throughout the world.

He had been a member of the Belgian Nat'l Committee for Crystallography since 1994 and he represented Belgium at many international congresses. On the way to ECM-20 in Krakow, he fell victim to an illness that, a year later, was to prove fatal. He accepted this without the slightest complaint.

We shall not forget the notable human quality of Ab Lenstra. His modesty prevented him from pushing himself. As a scientist he always sought after truth, a quality found also in his humanity where he was direct in word and deed.

The members of the Belgian Nat'l Committee for Crystallography and many others in the IUCr will continue to honour his memory.

Karl Michel

OBITUARY

Edward C. Lingafelter (1914-2003)

Prof. Edward Clay Lingafelter died on April 7 at the age of 89. His wife of 65 years, Roberta, preceded her husband in death by one day.

Ed was awarded the Ph.D. degree in chemistry by the U. of California at Berkeley in 1939 where he distinguished himself, gained a broad knowledge of chemistry, and developed an assured confidence when faced with un-anticipated questions. For example, when he was preparing for his Ph.D. qualifying exam, it was customary to schedule a preliminary meeting with the Advisory Committee to lay out for the candidate what would be expected in the exam. At this preliminary meeting, Ed was startled when the members of the committee began asking the tough questions expected on the qualifying exam itself. Ed recalled that on the very first question, he struggled to come up with a partial answer. Then, having gotten through that, he gained sufficient confidence to formulate a satisfactory answer to the second question and went on to an unqualified 'pass' of the exam! It remains uncertain whether Ed or the committee erred in their expectations for the meeting, but it seems unlikely, considering Ed's personality and character, that he misunderstood what the meeting was about. During his graduate studies at Berkeley, Ed became interested in X-ray diffraction and spent some time at the California Inst. of Technology in Pasadena where X-ray crystallographic studies were well advanced. This introduction proved to be a blessing for many of us who later had the good fortune to work for and with him.

After completing his studies at Berkeley in 1939, he located a temporary position in the Dept. of Chemistry at the U. of Washington in Seattle. Thus began his life's work. The appointment involved aiding Prof. Tarter in his studies on surfactants using classical physical chemical techniques. In view of Ed's interest in X-ray crystallography, he initiated diffraction studies on these compounds. To that end he was able to obtain the basic equipment for the study of single crystals. The equipment, mainly supplied by the California Inst. of Technology, was delivered in the late summer of 1942 and within weeks was producing beautiful rotation photographs of single crystals of long-chain sulfonates, detergents, whose properties were being studied by other means in the department.

Because of the very serious academic disruptions of World War II, the enrollment at the UW had decreased from about 11,000 in 1939 to about 4500 in 1945 at the end of the war. Thus it was that X-ray crystallographic studies could not continue until after the war. At the time, progress in molecular structure determination based on single crystal X-ray diffraction data was extremely slow because of the laborious computations, mainly by gear driven desk calculators. However, the era of electronic computers came to UW and to crystallography there in the early 1950s. The first crystallographic work was done on the accounting machines of the UW administration on a third shift arrangement. Soon after, however, Ed played a key role in acquiring the first electronic computers available to faculty and students at the UW. He was one of six members of a committee appointed by the Graduate School in the autumn of 1953 that arranged for an early IBM machine which became operational April 1, 1955. Then in 1957 it was replaced by the first stored program, drum memory, machine on campus, an IBM 650. This was about 1000 times faster than hand calculations. The IBM 650 was displaced in 1960 by the very large, at the time, IBM709 possessing 0.19 MBytes of memory and a 600 Byte operating system. Ed was active not only in acquiring these machines, but in supporting them from his research funds as each successive generation of machines came on line.

The early structures worked on at the UW were the sodium salts of n-alkane sulfonates and related paraffin-chain structures. During the decade of the 1950s, as more graduate students chose crystallographic problems, Ed's interests turned to the structures of metal complexes. Through the rest of his career, he and his students determined the structures of many organometallic complexes of both practical and theoretical interest. In this work he gave training and guidance to 39 graduate students and a score of post-doctoral students. The training in chemistry and crystallography was above reproach, but there were also great moments in the ethics of science. One memorable occasion was when, just as the UW group had managed to determine it, the structure of a zinc chelate appeared in *Acta Crystallographica*. At that time the group was in the process of checking a bond lengths and angles program. The bond lengths and angles reported in the paper were very different from those that Ed expected so the structure from the literature was used as a test case for the new program. The student doing the programming reported that something was wrong, he couldn't get the same results as those published. Ed sat down at the desk in his very characteristic way and looked at the results. In what seemed like an instant he said 'They've used β^* for β .' Then, instead of firing a letter off to the journal, he wrote to the author of the paper, pointing out the error, and suggesting they publish the correction as co-authors. It was a wonderful example of his magnanimous nature.

During most of his career, Ed carried a fairly heavy teaching load. He is remembered by his students as an inspiring lecturer, not only in crystallography, but also in other areas of chemistry as well. At the same time, he assumed rather heavy administrative duties, serving half-time as Assoc. Dean of the Graduate School of the UW from 1960-1969. His lectures, and his method of managing courses were always exceedingly well organized and he knew exactly the right level at which to 'pitch' a course. Therefore, he would go to the junior level physical chemistry class and then move into the Chemistry for Nurses class and get commendation from those disparate groups and then come back to the graduate students and shift attention appropriately. As his Berkeley exam foretold, he had the knowledge and gift to deliver the answers just right. But above all he cared about the training of students and his concern was palpable. For most of his career, Ed Lingafelter was active in the ACA, serving as President in 1974. He served as Co-editor of *Acta Cryst.*, 1975-1981, and on many committees for the Nat'l Science Foundation. He continued to be active in both teaching and research, reaching mandatory retirement in 1984 at the age of 70. Even after retiring, Ed continued in research as co-author on a number of papers and continued to help students and colleagues.

Jim Stewart, Lyle Jensen and Ron Stenkamp

In the memory of Ed and Roberta Lingafelter.



Edward Lingafelter and the late Luigi Sacconi activated, in the years 1964-1972, an outstanding NSF-CNR exchange program that allowed many to have a unique experience. At a time, when foreign research programs for pre-doctoral students were rare, the U. of Washington and U. of Firenze exchanged students each year in chemistry and crystallography. The American fellows had an opportunity to spend one year in Firenze, experiencing the strict rules in the lab of Prof. Sacconi, a world leader in coordination chemistry. At the same time, they enjoyed the glamour of one of the most beautiful cities that suffered, in those years, a dramatic flood.

The Italian post graduate students (there was no Ph.D. program in Italy at that time) had the privilege to spend one year on the beautiful campus of the U. of Washington where they could master the techniques of X-ray crystallography under the expert and paternal guidance of Ed Lingafelter. Structure

determination was giving a great impulse to the development of chemistry and they had the feeling of learning something very important. Seminars and group meetings were the occasion to appreciate Ed's charisma as a teacher. On weekends, Ed and Roberta and their five children hosted the students at their cabin in the woods. The long hikes in the Washington trails and the dinners in the house remain unforgettable. They loved to keep in touch with the pupils and their sound friendships have lasted over the years. Our small community shares feelings of indebtedness to Ed and to Roberta and deep sorrow for their simultaneous departure.

Carlo Mealli

OBITUARY

Henri A. Levy (1913-2003)



Henri A. Levy (B.S., 1935; Ph.D., 1938, Caltech) died on March 25, 2003 following a short illness. Born September 12, 1913 in Oxnard, California, he studied chemistry and physics at Caltech under Linus Pauling, staying on as a postdoctoral fellow in Pauling's lab after receiving his doctorate to begin his career in crystallography. In 1943, he moved to Oak Ridge Nat'l Lab (ORNL) where he continued research for many years, even after his initial retirement in 1975. Originally working on highly radioactive materials related to the war effort, he returned to studying the crystallographic structure of molecules following the war. Ernest Wollan and Clifford G. Shull had recently shown that neutron beams from the ORNL Graphite Reactor were diffracted by crystals in ways very similar to X-rays. Working with Selmer W. Peterson, he took advantage of the fact that neutron diffraction experiments could locate the positions of hydrogen atoms with much greater precision than X-ray studies. They took the lead in pioneering work on hydrogen containing crystals, such as potassium hydrogen fluoride, urea, maleic acid, and water (ice). The structures of all these materials involve significant hydrogen bonding. The unique properties of water and ice are largely the result of hydrogen bonding. Indeed, the Antarctic Place-Names Committee honored him, along with others who had worked on water and ice, by naming Levy Island in Antarctica's Crystal Sound after him. As the reactors at ORNL became more powerful and more sophisticated, he and his coworkers took the lead in developing computer-controlled instruments for making diffraction measurements, and they developed computer programs for processing the data. The experimental and computational methods that they developed have had a profound impact on the way structures of large molecules are studied today. Following his official 'retirement' in 1975, he continued research as a consultant to ORNL and as a Professor at the U. of Tennessee. During this time, he turned his attention to solving the three-dimensional structure of large biological molecules, devoting much of his efforts to tomography of electron microscopic images of transcribing and replicating chromatin, in collaboration with Don and Ada Olins. He belonged to numerous professional societies, serving as President of the ACA in 1965 and as a delegate to the IUCr for several years.

David Levy and Bill Busing

OBITUARY

Mary E. Mrose (1912-2003)

Mary E. Mrose, was a mineralogist, crystallographer and a teacher. She was also a bonsai enthusiast for whom the International Pavilion at the National Bonsai and Penjing Museum is named. She was born in 1910, one of eight children of Emil W. and Mary M. Mrose. Her first career was that of teacher. After certification from the State Normal School at Salem, Massachusetts in 1931, she taught history, geography and civics, and occasionally mathematics and English at the junior high school level. While teaching, she earned an M.A. in Geography and a B.S. in Education. She also studied at the New England Conservatory of Music and became an accomplished pianist. Moving toward her second career, Ms. Mrose studied geology. In the 1940s, after a year's stint as an industrial chemist, she taught geology at Boston U., at the same time serving as research assistant in the Harvard Dept. of Mineralogy. There she was involved in the preparation of Volume 11 of the 7th edition of Dana's System of Mineralogy, the bible of the field.

Her second career began in earnest in 1953, when she joined the US Geological Survey in Washington, D.C. Until her official retirement in 1983, her activities included X-ray studies of minerals; field work in many parts of the US; and authorship or co-authorship of seventy three articles, including papers in which she described and named nineteen new minerals. One of many honors and awards bestowed upon her was the designation of a very rare mineral from Montezuma, Mexico, as 'Mroseite' in recognition of her valuable contributions to mineralogy. She was an active member of the Int'l Centre for Diffraction Data for thirty years and was a member of mineralogical and geological societies in the USA, Canada, Great Britain, Ireland and France.

Her third career, which began after her retirement from the Geological Survey, was with the Nat'l Inst. of Standards and Technology where she compiled data for an update of Crystal Data: Determinative Tables and a companion database, which was published by the Int'l Center for Diffraction Data.

David Garvin & Mary Ann Orlando (September 1995)

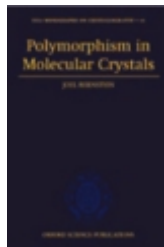
Beyond 1995 things pretty much remained the same for her until her macular degeneration stopped her from driving. She also was a source for Polish recipes. She was so excited when someone brought her some pigs feet so she could make her special 'cold feet' (I can't begin to reproduce the Polish name). She never missed Wall Street Week on PBS and she certainly could wax indignant about current affairs! Her generosity is legend and her spirit was indefatigable. Her body may have deserted her but she was mentally sharp as a tack and was fun to talk to right up to the end.

Judy Konnert (April, 2003)

BOOK REVIEW

Polymorphism in Molecular Crystals

Joel Bernstein, Clarendon Press, Oxford, May, 2002, Hardcover, ISBN 019 850605 8.



The latest Oxford Science Publication in the IUCr series of Monographs on Crystallography. The book has 410 pages plus 14 pages of Contents and Author's Preface and over 200 line-drawn figures and schemes. The scientific community has been presented with a long-awaited book on polymorphism. It comes from a world-renowned expert in this field, Joel Bernstein (Ben-Gurion U., Beer Sheva). His three-decade long scientific interest in polymorphs has been marked by many well known achievements such as descriptions of conformational, disappearing or concomitant polymorphs and jumping crystals, as well as development of graph descriptors for hydrogen-bonded patterns commonly used for comparisons of molecular aggregation, particularly in polymorphs.

Personally, I was already excited by the titles of sections and subsections in the Contents. Then I 'swallowed' all the chapters one by one in a few days. The scope and purpose of the book are outlined in the Introduction. Obviously he had to make choices from the thousands of substances referred to as polymorphs in literature, to which related subjects should be included and, even more importantly, which of many definitions of polymorphism to accept. His decision to take the least restrictive approach of supramolecular isomorphism was a good one. Although written by a chemical crystallographer mainly for chemists, crystallographers, material scientists and pharmacists, the book will also appeal to specialists in related sciences. It is written in an easy style that takes us back to the first observations of polymorphism and follows its history up to the present.

Over the last decades the subject has constantly become more of a concern to the scientific community. Any scientist involved in crystallography, materials sciences, solid-state physics, chemistry or pharmacology, must be aware of the possible polymorphic modifications of any given substance. No type of compound is exempt, polymorphs occur among small-molecules, medicinal drugs, pigments, explosives, fats, charge-transfer complexes, inclusion compounds, polymers and proteins. The different properties of polymorphs make the subject ideal for studying structure-property relationships, and essential, or even obligatory, for technological applications in chemistry-related industries. Polymorphs may differ in color, therapeutic activity, thermal or electric conductivity. Even fats in chocolate may melt and taste differently. Bernstein's book is a rich and comprehensive compilation and illustration of the structural variety of polymorphs and their properties.

There is also a chapter on legal issues related to polymorphs in industry, and litigations over the patent protection of medicinal drugs. The book can be recommended for all researchers working on organic materials, or any materials indeed. It will be of interest to academic lecturers, who will find additional illustrations for their lectures, and to undergraduates studying structural or materials sciences. The huge list of about 1500 references to scientific articles, conveniently cited with their titles, guides the reader to original and complementary sources. Page numbers added to references, direct one back to where they are cited. The Index (10 pages), also facilitates reading and quick location of a subject of interest. Today's instrumentation and powerful computers make it possible to rapidly perform structural analyses at various temperatures and even to do charge density studies of proteins. Powder diffraction

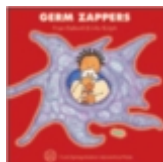
experiments resolve two or more phases of increasingly complex substances, while theoretical predictions of the crystal structures become more efficient. With these facilities at hand, appropriate education and awareness of polymorphism is crucial. Today's knowledge of the field of polymorphism appears as the tip of an iceberg, and Bernstein declares that one purpose of his book is to be a platform for future research. 'Be wary of the polymorph, that slyly lies in wait' in your laboratory, and its scientific and economic implications!

Reviewed by Andrzej Katrusiak

BOOK REVIEW

Enjoy Your Cells, Have a Nice DNA, Gene Machines, and Germ Zappers

All four by Fran Balkwill and Mic Rolph, published by Cold Spring Harbor Laboratory Press (2002), paperback and hardcover.



These four books are aimed at a youthful audience of around 9-12 years of age. The topics covered include different types of cells and the structure of DNA. DNA is a recurring topic, of course. The first three books are somewhat similar in fact because DNA figures prominently in each of them. Each book, however, examines a different aspect of DNA including its role in protein synthesis, cell division, reproduction, and growth and development of organisms. Germ Zappers is significantly different, covering the subject of the immune system.

The science content of the books comes from Fran Balkwill, Prof. of Cancer Biology at Barts and the London Queen Mary's School of Medicine and Dentistry. Illustrations are the work of Mic Rolph, a graphic designer and illustrator. The books are designed to hold a pre-adolescent's attention while providing some pretty amazingly detailed science. Who knew that dendritic cells alerted the mighty lymphocyte squads? Or that the 'Natural Killer' cells were a little like Dirty Harry ('make my day' considering their gratuitous ventilation of infected cells)? Mic Rolph's illustrations show his skill in drawing everything from menacing bacteria to babies, young people, dinosaurs, and the comparative insides of mice and humans.

This reviewer enjoyed the task of reading these books and recommends them highly to anyone who knows of a receptive reader, whatever the age.

Reviewed by Paul Anderson

IUCR ACTIVITIES

XX Congress IUCr and General Assembly Update



At the end of March 2003, the Italian organizers of the XX IUCr Congress (Florence 2005) invited the President of IUCr (William L. Duax) and the Chair of the subsequent Nagoya Congress (Yasuhiko Fujii) for a short visit. All of the practical and scientific aspects of the organization were jointly discussed with the Scientific and Local Chairs (Carlo Mealli and Paola Paoli) and other Italian representatives who have responsibilities in the international crystallographic community, Paola Spadon (President of AIC), Davide Viterbo (IUCr Executive Committee Member), and Giuseppe Filippini (Secretary of ECA). The work done up to date regarding the nomination of the Scientific Program Committee and many other organizational issues was presented to the guests. The group subsequently visited the Conference venue and looked around the conference areas which Duax agreed were excellent. Having previous experience as Program Chair of the XXVII IUCr in Seattle he offered a lot of useful advice and warnings on how to best use all the facilities.



Seated from the left, Yasuhiko Fujii, Carlo Mealli, Bill Duax, Davide Viterbo and Leonardo Sorelli. In the mirror from the left, Giuseppe Filippini, Lorenzo Mori and Paola Paoli.

During their stay in Florence, the guests visited the new Campus of the U. of Florence and in particular the X-ray facilities of the crystallographic center (CRIST). Prof. Duax was also invited to the Magnetic Resonance Lab, CERM, directed by Ivano Bertini, where he presented a seminar about his recent research on the Evolution of the Genetic Code.

The two guests also found a little time to enjoy some of the more renowned tourist attractions of Florence (a guided tour of the Uffizi Gallery, for instance). Moreover, they agreed that Italian food and wines will certainly be an extra bonus in attracting a large number of crystallographers to Florence in the year 2005.

Carlo Mealli and Paola Paoli

Please note the new address for Carlo Mealli

ICCOM - CNR

Via Madonna del Piano s.n.c.

50019 Sesto Fiorentino (Firenze), Italy

Tel. 0039 055 5225884 FAX 0039 055 5225203 e-mail: Carlo.Mealli@iccom.cnr.it