

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



W. L. Duax

The XXth Congress and General Assembly of the IUCr in Florence in 2005 will surely be one of the most exciting and successful meetings in our 50-year history. Carlo Mealli and the members of the scientific program committee have issued a call for suggestions for plenary lecturers, microsymposia topics and microsymposia chairs. The program committee members are drawn from the Commissions of the Union and all National Committees have been asked to submit suggestions for the program. Suggestions are also welcome from individual crystallographers everywhere. Please exercise your right to participate in the affairs of the union. Write to Carlo or any member of the program committee with your program suggestions.

The Congress in Florence will provide a venue for the members of the Commissions of the Union to gather, plan and coordinate their activities, and appoint new members and chairs. The Commissions rely upon dynamic, imaginative and hard working members in order to prosper and serve the community. All the National Committees of our 40 member countries have been invited to nominate individuals for membership on the commissions. Your input in this process is vitally important. If you are willing to serve on a committee or wish to nominate someone else for such a post, contact a member of the National Committee in your country, expressing your thoughts.

Finally, there will be the usual turnover in the membership of the Executive Committee in Florence. A call for nominations for the position of President of the IUCr and other vacancies to be filled has been extended to all National Committees. If you have any suggestions, contact a member of the National Committee in your country. As soon as nominations for membership on the Executive Committee are received, they will be posted on the IUCr website.

This Newsletter is distributed to 15,000 individuals worldwide. However, there are only 9928 crystallographers listed in the IUCr World Directory and there are many countries in the world that do not receive any copies of the Newsletter. A list of countries in which fewer than 5 newsletters are distributed appears on Page 8. If you know of a scientist (ideally, a crystallographer) in any of these countries, please send his or her name and address to the IUCr Newsletter office so that we can add that person to the mailing list and write to them and ask about sending copies for distribution to appropriate institutions and libraries.

When the World Directory was assembled with assistance of regional editors, the total number of registered crystallographers reached 7959 (10th edition). The transition to an electronic directory, for which individuals were responsible to register, reduced the number of crystallographers who have updated their entry to 5840. If you are now or ever have been a crystallographer or have consorted or coauthored a paper on some aspect of diffraction, and you are not currently listed in the World Directory of Crystallography, please register. Instructions appear on page 30.

One major impediment to participation by many countries not currently in the Union is the cost of membership. While the cost is relatively low, it is not easy for crystallographers in some countries to identify a source of continuing annual support. In fact, political change and economic setbacks have made it difficult for some member countries to maintain their membership. Economic difficulties in Argentina and the Ukraine have jeopardized their continued membership.

When the question of suspension of the membership of Argentina and the Ukraine was brought before the general assembly in Geneva, the delegates voted to allow Argentina and the Ukraine to continue as non-voting members. Crystallographers in Argentina have since convinced government representatives of the importance of IUCr membership and obtained a commitment to pay current and future dues. However, the Argentinian government would not accept responsibility for payment of past dues. Because the IUCr bylaws require payment of past dues before current dues, some special action was required. I am pleased to say that the Spanish National Committee, the US National Committee and the American Crystallographic Assn (an IUCr regional affiliate) agreed to contribute equally to pay the back dues for Argentina so that they could be reinstated as voting members.

It may be appropriate to review the IUCr bylaws governing membership in order to address such problems in the future and to find ways to expand the membership of our Union to include all countries where diffraction physics and X-ray crystallography are conducted. The suggestions put forward so far have been a) to have a limited time non-voting, no cost membership, b) to establish a sliding scale for membership dues tied to an economic barometer (i.e. gross national product or the average salary of crystallographers in the country), c) membership in a Regional Affiliate (AsCA, ECA, ACA) that would allow a country to send a non-voting delegate to the Congress, and/or d) create a fund specifically for assistance to countries in need (similar to the fund established by the ACA for its Latin American Initiative). Any of these options might be an intermediate step towards full membership and participation. Delegates to the XXth Congress may wish to place matters such as this on the agenda.

Bill Duax

duax@hwi.buffalo.edu

LETTER TO THE EDITOR

50 years of DNA continued

Mark Spackman's commentary on the origins of the DNA structure paints a somewhat simplistic picture of what I understand to be the background to Watson and Crick's 1953 Nature paper. Whilst it is true that 'No (basic) crystallographic information is presented (in the actual paper) and no crystallographic experiment was reported..' the whole thing is based largely on crystallographic results..... **from other groups!** Indeed around that time modelling DNA seems to have been a very prevalent occupation in many laboratories. They were all based on very crude fibre diffraction X-ray photographs which contained very little detail. The Watson and Crick model turned out to be the best at that time but was not properly validated until high resolution structures from single crystal analogues were produced (eg Lisgarten *et al*, *Nature Structural Biology*, 2002, **9**, 57-60).

1) Watson and Crick were very much aware of the papers being prepared by members of the King's College, London, group and Watson in particular visited Maurice Wilkins' laboratory several times during the run up to the building of the structure model and writing the paper with Crick. They did not in fact need to be aware of the fine details provided in the 'following communications', only the basic parameters of the helix, a knowledge of stereochemistry and base pairing in DNA, and the inspiration, as the cartoon below shows, to build a double helical model (other groups had tried single and triple stranded models).



2) *Nature* has always been known as the elite publishing medium for a broad spectrum of current topics and it is inconceivable that the journal would publish 'little more than a hypothetical structure'. It is no coincidence that the three papers mentioned by Professor Spackman were published concurrently in *Nature* and one must conclude that this was an editorial decision and the editor did in fact recognise the importance of the interactions of this trilogy of papers. Nowadays groups tend to publish joint papers, with large numbers of co-authors, in order to strengthen the arguments presented. Apparently this was not so back in the 1950's.

3) The question as to 'leaving to you to decide whether the Watson & Crick model could have been devised while being 'not aware of the details' of the crystallographic results' **does not arise**. James Watson in his own account of the discovery of the DNA structure 'The Double Helix' (Weidenfeld and Nicolson, 1965, London) explains in some detail how it was accomplished. On p172 Watson says 'I started to run through the (known) details of the B form (of DNA) (subject of the famous Rosalind Franklin X-ray diffraction pattern)....the evidence (was) that DNA was a helix which repeated its pattern every 34Å along the helical axis.' On page 175 'Especially important was the meridional reflection at 3.4Å, much stronger than any other. This could only mean that the 3.4Å-thick purine and pyrimidine bases

were stacked on top of each other in a direction perpendicular to the helix axis'. [Whilst this of course could not be proved, this vital feature of the model was not simply hypothetical but based on an experimental fact which had already been used by Astbury] 'In addition we knew from both electron-microscope and X-ray evidence that the helix diameter was about 20Å.' Another vital model parameter based on measurement.

Hence the basic geometry of the model depended upon known experimental evidence, albeit not measured by Watson and Crick *per se*.

The DNA model building itself which was designed to be in keeping with stereochemical principles, depended strongly on several other factors, all experimentally derived:

- (a) The geometry of cytidine determined by the **crystallographer** Sven Furberg.
- (b) The nature of the base pairing (Chargaff's rules).
- (c) The possible base pairing H-bonding patterns and their geometry. This could be derived from a **wealth of crystallographic data**, and was revealed to Watson and Crick by Jerry Donohue, a renowned world expert on H-bonding in 1953.

The Watson and Crick model whilst being somewhat rough and ready was consistent with the main features of the B DNA fibre diagram. Ironically Rosalind Franklin from King's College, and afterwards Birkbeck College, London University had better, more detailed data, derived from her beautiful DNA photographs and was working towards a more conventionally derived model, using Patterson functions, but was unable to complete this work due to her fatal illness ('Rosalind Franklin, the Dark Lady of DNA' by Brenda Maddox, Harper Collins, 2002, is a very good read). Other workers had of course tried unsuccessfully to derive DNA models, including Astbury, Furberg, and Linus Pauling. Watson and Crick's model has stood the test of time, including several periods when it came under severe criticism, and is now generally accepted as being essentially correct. As revealed in a BBC documentary Watson and Crick did fail to include some of the finer details and were criticised by Rosalind herself for excluding the biologically important water molecules.

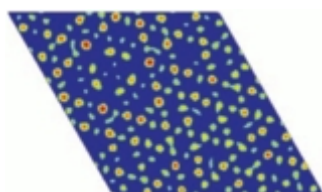
Rex Palmer, Birkbeck College, London

IUCR JOURNALS NEWS

Three-dimensional reconstruction of the ν -AlCrFe phase by electron crystallography

Three-dimensional reconstruction of the ν -AlCrFe phase by electron crystallography

***Acta Cryst.* (2003). A59, 526-539**

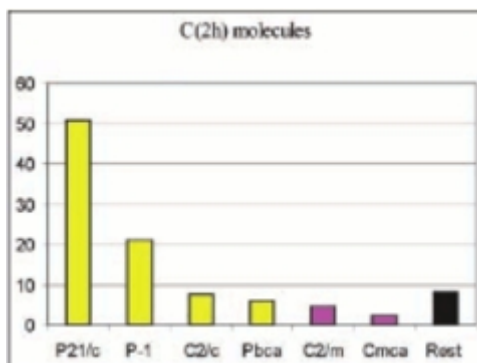


A section of the 3D potential map of ν -AlCrFe obtained by electron crystallography. All atoms are clearly resolved and it is possible to distinguish transition metals (Fe, Cr, strong peaks) from Al (weak peaks). The most complicated crystal structure ever solved to atomic resolution by electron crystallography is presented in this article. Because of the huge unit cell (ν -AlCrFe, $P6_3/m$, $a = b = 40.7 \text{ \AA}$, $c = 12.5 \text{ \AA}$), it was necessary to combine crystallographic data from 13 projections to resolve the atoms. Electron microscopy images containing both amplitude and phase information were combined with amplitudes from electron diffraction patterns. 124 of the 129 unique atoms (1176 in the unit cell) were found in the remarkably clean calculated potential maps – see figure. This investigation demonstrates that inorganic crystals of any complexity can be solved by electron crystallography.

X. D. Zou, Z. M. Mo, S. Hovmöller, X. Z. Li and K. H. Kuo

A database survey of molecular and crystallographic symmetry

Acta Cryst. (2003). B59, 634–640



Histogram showing the distribution of the molecules of C_{2h} ($2/m$) symmetry over space group and Wyckoff position. The colours of the bars indicate the symmetry of the Wyckoff position, yellow: C_i (1) pink: C_{2h} ($2/m$).

The point of contact between molecular and crystallographic symmetries is that of the Wyckoff position, the position at which a molecule resides in a crystal structure. The Wyckoff position may have the same symmetry as the molecule, may have some symmetry in common with the molecule or may have no symmetry at all. Analysis of thousands of crystal structures, using the relational database CSDSymmetry, has led to the tabulation of the occupancies of Wyckoff positions in crystal structures, the collation of the most favoured locations for a molecule of a particular point-group symmetry in terms of Wyckoff position and space group, and the observation of a hierarchy in the degree of retention of molecular symmetry.

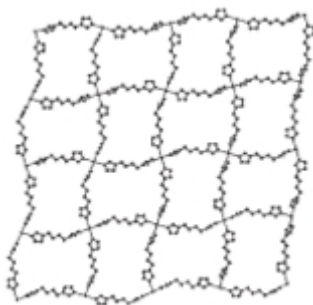
E. Pidcock, W. D. S. Motherwell and J. C. Cole

IUCR JOURNALS NEWS

A novel Cd^{II} coordination polymer with 1,1'-(1,4-butanediyl)diimidazole

A novel Cd^{II} coordination polymer with 1,1'-(1,4-butanediyl)diimidazole

Acta Cryst. (2003). C59, m482-m483



The two-dimensional sheet of the (4,4)-network.

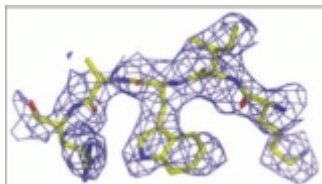
The research in coordination polymers has been rapidly expanding because of their fascinating structural diversity and potential applications as functional material. Much of the work has so far been focused on coordination polymers with rigid ligands. This paper reports on the preparation and crystal structure of a Cd^{II} coordination polymer with a flexible ligand 1,1'-(1,4-butanediyl)diimidazole (*L*). The Cd^{II} cation occupies the inversion centre, and is six-coordinated by four nitrogen atoms from four *L* molecules, and two chloride anions. Each *L* molecule coordinates to two Cd^{II} cations through its two aromatic nitrogen atoms acting as a bridging bidentate ligand. The Cd^{II} cations are bridged by four *L* molecules to form a two-dimensional neutral (4,4)-network. The square-grid sheets superpose in an off-set fashion.

J.-F. Ma, J. Yang and J.-F. Liu

IUCR JOURNALS NEWS

Away from the edge: SAD phasing from the sulfur anomalous signal measured in-house with chromium radiation

***Acta Cryst.* (2003). D59, 1943-1957**



Experimental electron-density map of thaumatin for the region including Trp51 generated from data collected with Cr $K\alpha$ data to 3.0 Å resolution and sulfur SAD phases.

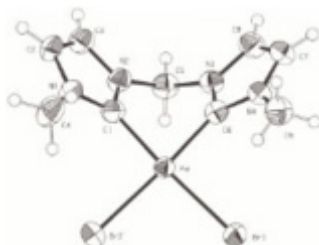
The solution of protein structures using the anomalous scattering from sulfur in native proteins (S-SAD) is becoming more widespread. Most often Cu $K\alpha$ ($\lambda = 1.5418$ Å) radiation is used, for which Δf for sulfur is 0.56 electrons. The authors have developed a system for the home laboratory employing Cr $K\alpha$ radiation ($\lambda = 2.2909$ Å) which doubles the anomalous signal from sulfur to 1.14 electrons. The authors describe the hardware and software tools necessary to take advantage of this enhanced anomalous signal in the test proteins thaumatin and trypsin. The results show that interpretable maps can be generated in the resolution range 3.5–2.8 Å using much less data than required for Cu S-SAD. Caveats associated with the experiment, radiation damage and absorption, are described; solutions to these caveats are also provided.

C. Yang, J. W. Pflugrath, D. A. Courville, C. N. Stence and J. D. Ferrara

IUCR JOURNALS NEWS

Dibromo(1,1'-dimethyl-3,3'-methylenediimidazoline-2,2'-diylidene)palladium(II)

***Acta Cryst.* (2003). E59, m970-m971**



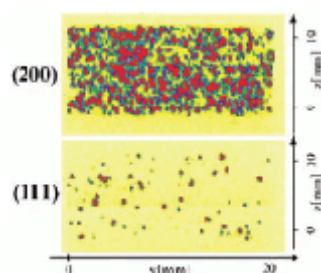
The perspective view of the title compound.

The catalytic properties of *N*-heterocyclic carbene (NHC) complexes for various reactions are currently being investigated by many groups worldwide. This paper presents the structure of dibromo(1,1'-dimethyl-3,3'-methylenediimidazoline-2,2'-diylidene)palladium(II), a complex that is so active in the Heck reaction that it even activates chloroarenes. In the course of the research program on the methane activation it was found that these NHC complexes show a surprisingly high stability towards strong acids. For the catalytic activation of methane in trifluoroacetic acid the title complex has been shown to be the most active NHC complex; a methane conversion of up to 4.3% could be accomplished.

E. Herdtweck, M. Muehlhofer and T. Strassner

Texture and microstructure imaging in six dimensions with high-energy synchrotron radiation

J. Appl. Cryst. (2003). **36**, 1240-1255



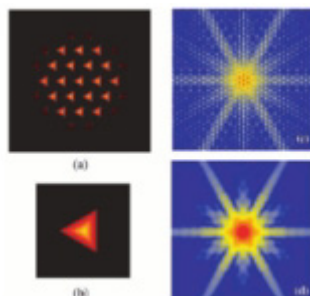
Projections (in sheet normal direction x) of grains of a recrystallized nickel sheet with cube texture. The technique visualizes only those grains that have either a $[200]$ or a $[111]$ direction (nearly) parallel to the rolling direction z of the sheet. Other groups of grains can be elected as well, by using other lattice planes and/or irradiating the sample in other orientations.

Texture and microstructure of a polycrystalline material are characterized by specifying the positions and orientations of all crystallites in the six-dimensional orientation-location space $\{\phi_1 \Phi \phi_2 xyz\}$. Two-dimensional sections and projections of this space can be imaged by the diffraction of hard synchrotron X-rays ($\sim 0.1 \text{ \AA}$) using a 'moving-area-detector' technique combined with either a diffraction-angle or a diffraction-plane slit. Since the X-ray beam 'sweeps' continuously over the sample coordinates, the extremely high orientation- and location-resolving power of synchrotron radiation can thus be fully exploited. The technique can be used to measure the 'field' of local textures, or the 'orientation stereology' of the individual grains, in the bulk of even big samples, with penetration depths comparable to those of neutrons.

H. J. Bunge, L. Wcislak, H. Klein, U. Garbe and J. R. Schneider

Imaging of quantum array structures with coherent and partially coherent diffraction

J. Synchrotron Rad. (2003), 10, 409–415



A 2D array of quantum dots (a), shape of individual island (b) and corresponding coherent diffraction patterns (c, d).

Quantum structures on the nanometer scale are important elements of modern technology. Their electronic properties directly depend on the structure of these devices. We propose to use the technique of coherent X-ray diffraction in combination with phase retrieval methods based on the Gerchberg–Saxton–Fienup algorithm to image quantum dots in a model-independent way. An image of a quantum dot array and its diffraction pattern is shown to the right. We have shown that the correct shape and orientation of the individual island can be obtained in the case of coherent illumination. We also demonstrated the possibility of imaging individual islands with partially coherent illumination when the coherence length of the incoming beam is reduced to match the size of the island.

I. A. Vartanyants and I. K. Robinson

IUCR ACTIVITIES

CIFNEWS-9: New CIF dictionaries and International Tables Volume G



I.D. Brown

The publication of Volume G of International Tables for Crystallography, scheduled for 2004, will provide crystallographers with a comprehensive description of the CIF project ranging from an account of its history and philosophy to details of all the approved CIF dictionaries. It will answer all the questions you ever had about CIF and even questions you probably never thought of. Each of the CIF dictionaries will be accompanied by an article outlining the rationale for the choice of the items that are included and how these are organized, making this volume the complete reference source on the topic.

To ensure that this volume is as current as possible, COMCIFS has been working hard to update the suite of CIF dictionaries before the copy deadline. Consequently this past summer has seen the approval of a new dictionary and the revision of two others. These dictionaries can be viewed on the IUCr web site, www.iucr.org, in a variety of formats. The canonical version of each dictionary is an ASCII text file using the STAR syntax (the same syntax as is used in CIF). This version has the complete text and is the one used as input to CIF applications, such as the recently released editor and browser CIFEDIT [Toby (2003), *J. Appl. Cryst.* **36**, 1288-1289]. The other formats in which the dictionaries are presented, such as html and pdf, are designed to make the dictionaries easy to read.

The `cif_core` dictionary will be familiar to anyone working in small-cell crystallography (inorganic and small molecule compounds). It is the preferred format for publication of structure determinations, and it is increasingly being adopted for the interchange of crystallographic information between applications. Its widespread use over the past 10 years has revealed areas where improvements and additions are needed. As a result the `cif_core` dictionary is currently undergoing a major review which will continue well into 2004. The recently approved version 2.3 contains some of the less controversial proposals. These include the replacement of the `_symmetry` items by a more systematically defined set of `_space_group` items from the newly adopted symmetry CIF dictionary. Other changes include the addition of items to permit the Cambridge Crystallographic Data Centre to provide a CIF output from the Cambridge Structural Database. Still to come are items that will describe crystal twinning and the chemistry of molecules. Further information is available at www.iucr.org/iucrtop/cif/cif_core/index.html and the dictionary itself can be downloaded from ftp://ftp.iucr.org/pub/cif_core_2.3.dic.

ImgCIF is used for recording images, specifically the two-dimensional images of diffraction patterns that are now being routinely measured. This dictionary defines the items used in the ASCII version of an imgCIF as well as its isomorphous Crystallographic Binary File (CBF). The primary purpose of the `cif_img` dictionary is to extend the `cif_mm` dictionary to allow CIFs to record synchrotron diffraction images for structural biology. Writing applications using this dictionary revealed the need for a number of technical changes and these have been included in the recently approved version 1.3.1. Further information can be found at <http://www.iucr.org/iucr-top/cif/imgcif/index.html> and the canonical ASCII version of the dictionary is available from ftp://ftp.iucr.org/pub/cif_img_1.3.1.dic.

A new dictionary, `cif_rho_1.0`, has also been added to the suite of approved dictionaries. It is designed to archive electron density (ρ) measurements using the multipole expansion model proposed by Stewart

[(1973), *J. Chem. Phys.* **58**, 1668] and developed by Hansen and Coppens [(1978), *Acta Cryst.* **A34**, 909-921]. It is a relatively small dictionary designed as a supplement to the cif_core dictionary. Further information is on the rhoCIF home page www.iucr.org/iucr-top/cif/rho/index.html. The canonical ASCII version of the dictionary can be downloaded from [ftp: //ftp.iucr.org/pub/cif_rho_1.0.dic](ftp://ftp.iucr.org/pub/cif_rho_1.0.dic).

David Brown, Chair, COMCIFS

MISCELLANY

Countries that receive less than 5 issues of the IUCr Newsletter

ALBANIA
BELARUS
BURMA
CENTRAL AFRICA
ERITREA
FIJI
ICELAND
IRAQ
KUWAIT
LITHUANIA
MOROCCO
PERU
PHILIPPINES
REP OF GEORGIA
REP OF KOREA
REP OF TADJIKISTAN
SAUDI ARABIA
SRI LANKA
TAHITI
TRINIDAD WI
TUNISIA
TURKMENISTAN
UNITED ARAB EMIRATES
URUGUAY
YUGOSLAVIA
ZIMBABWE

MEETING REPORT

ECM-21**Durban, South Africa, August 2003**

The 21st European Crystallographic Meeting was held at the International Convention Center (ICC) in Durban, South Africa, and was attended by over 500 official delegates and 50 accompanying persons from 49 countries, making it the largest gathering of crystallographers in Africa to date. Approximately 100 students and younger scientists were able to attend as a result of sponsorships from particularly the IUCr, ECA, South African NRF and the South African government (DTI and DACST).

ECM-21 was preceded by two satellite meetings: INDABA 4 in Skukuza, Kruger National Park (August 18-22, Chair: P. van Rooyen, Pretoria), and the African Neutron Diffraction Meeting (ANDM) at Amanzingwe, near Pretoria (August 20-22, Chair: A. Venter).



ECA prize lecture laureate: Carmelo Giacovazzo (front, left), with Jan Boeyens, Chair: Programme Committee, and Claude Lecomte, President: ECA, and back row: Davide Viterbo, IUCr Exec Committee. ECM-21 started with three workshops, Powder and Single Crystal Crystallography (PSCC; Chair: L. Cranswick), Protein Crystallography (E. Dobson) and the Cambridge Structural Database (K. Lipscomb). These were attended by approximately 100 delegates and students, the PSCC workshop attracted about 70 individuals!

C. Lecomte, President of the European Crystallographic Assn (ECA) formally opened ECM-21 on Sunday evening, attended by different guests of honor, including W. Duax, President of the IUCr, and Mayor Mdladla, of the greater Durban Municipality (eThekweni), who also hosted the opening mixer.

On Monday evening, C. Giacovazzo (Bari, Italy) received the ECA Prize from the President for his contribution towards crystallography. Carmelo then delivered the prize lecture 'Phasing powder data, small- and macro-molecules: a unique project'.



At opening Mixer: Gideon Steyl (RAU, Joburg) with Ake Oskarsson (Lund, Sweden: Program Committee member) and his wife, Christina.

The Program Committee, chaired by J. Boeyens (Pretoria, SA) organized a splendid program, consisting of eight plenary lectures: 'Drug targets in tropical diseases' (W. Hol, Seattle, USA); 'Structure determination from powders: crossing the 100-atom threshold' (B. David, Chilton, UK); 'High-throughput structural biology and drug discovery: Challenges and Opportunities' (T. Blundell, Cambridge, UK); 'Quasicrystals' (T. Janssen, Nijmegen, The Netherlands); 'The wonderful world of crystal structures of sulfosalts' (E. Makovicky, Copenhagen, Denmark); 'Tools for mineralogical crystallography' (G. Artioli, Milano, Italy); and 'Measuring and modelling atomic and magnetic disorder in crystals' (R. McGreevy, Chilton, UK). Unfortunately the final plenary lecture had to be changed due to Prof Ossipyan falling ill, and we were treated to an excellent talk by J. Bernstein on 'Chemistry in the Courtroom'.

Approximately 200 talks from 46 microsymposia in five focus areas (Biological and Macro-molecular Crystallography, Materials and Minerals, Experimental and Computational Techniques, Chemical Crystallography, Special Techniques) ran over four days. Students, young scientists and established senior people had the opportunity to present their science, and a significant amount of high quality science was presented.



Mayor Mdladla and Bill Duax at the opening Mixer.

Sponsorships provided a backup to the meeting, although it was a bit disappointing that both larger South African and European companies were reluctant to contribute to the meeting – even by just sponsoring individual students from Europe. Nevertheless, the main sponsors of the meeting ensured that we could provide necessary administrative backup to have a successful conference. These sponsors are specifically thanked for these valuable contributions. Furthermore, last minute sponsors for refreshments are also thanked for ensuring that delegates were not overcome by thirst during the poster sessions and tea/coffee breaks in the hot Durban climate.

There were sixteen exhibitors, including stands from our sponsors. We are particularly thankful for all the companies that exhibited to ensure that delegates could access first-hand information on new equipment developments.

Two poster sessions were held on Tuesday and Wednesday afternoons. All posters were displayed for the whole meeting to ensure maximum exposure and interaction between delegates. Although being a bit more demanding on infra structure, in general very favourable feedback on this poster session format was received from the delegates.

ECM-21 was organized by the South African Crystallographic Assn (SACrS), under the auspices of the ECA, and the general commercial aspects were handled by Conference Call, headed by L. Volker. The website and Abstract book were the responsibility of D. Billing (Wits), D. Liles (Pretoria), M. Fernandez (Wits) and J. Dillen (Stellenbosch). Both groups need a special word of recognition for streamlined work and continued dedication.

The closing ceremony and banquet was held on Thursday evening in a large Marquee tent, delegates enjoying a selection of 'spit' barbequed meats and wines amidst traditional Zulu and African Latin dances. Many delegates used the opportunity to try their Zulu war dance techniques, with limited variations of success.



Quenching their thirst after viewing game: Andre' Roodt (Joburg), Peter Comba (Heidelberg, Germany), Marlene Linde (RAU, Joburg),

Six poster prizes were awarded to the following authors (only those presenting are listed) during the closing ceremony: IUCr Prize: R. L. Owen (Oxford, UK), 'Birefringence in Protein Crystallography'; PDB Prize: C. M. C. Lobley (Cambridge, UK), 'Structural Studies of the Enzymes of Pantothenate Synthesis'; Oxford Cryosystems Prize: K. W. Törnroos (Bergen, Norway), 'Ordering in a spin crossover compound – uncovering the nature of the intermediate phase of iron(II) tris(2-picolyamine) dichloride ethanol solvate'; Cambridge Structural Database (three prizes): T. Aree (Bangkok, Thailand), 'A new crystal form of cyclodextrinethanol inclusion complex', A. Docherty (Glasgow, UK), 'Accuracy in structure determination from powder diffraction data by simulated annealing', and T. le Roex (Cape Town, South Africa), 'Structure and kinetic reactivity of a diol host compound'.

During the closing banquet J. Boeyens gave a brief overview of some aspects of South African Crystallographic history with details on some of the interesting and eccentric people who contributed toward establishing the community here.



Disembarking from game viewing vehicle at Tala game reserve: Leo Kirsten (Joburg) with Elena Boldyreva (Novosibirsk) and Emil Makovicky (Copenhagen, Denmark) in background.

The delegates were given the opportunity to put on their safari jackets to prepare for the game park trip on Friday to Tala Game lodge. They had the opportunity to see different game, the 18 giraffe specifically 'standing out' as well as the close-up on rhinos, and for those who were lucky, appreciating the hippo when the lazy-looking creatures showed a bit more body from the muddy water.

Unique difficulties were experienced with regard to the budget, and eventually it had to be tightened significantly. Thus, we are especially grateful to sponsors committed from the beginning to support us, but also late sponsors enabling a continuous flow of delegates in the exhibition area, without whom we would have struggled to make ends meet.

Andreas Roodt, Chair: OC: ECM-21

MEETING REPORT

2003 CrSJ Annual Meeting



The 2003 Annual Meeting and General Assembly of the Crystallographic Society of Japan was held in Kumamoto, Japan, in December 2003. It was attended by 480 people and included 2 symposiums, 71 oral presentations and 172 poster presentations covering all aspects of crystallography, and an industrial exhibition.



Y. Fujii (IUCr2005 Program Committee), M. Sakata (Program Chair of AsCA'04), Y. Ohashi (EC of IUCr), Y. Yamagata (Chair of CrSJ'03 Kumamoto), S. Sasaki (Chair of National Committee for Crystallography), and J. Akimitsu

The two symposiums were on 'Nano technology and crystallography' and 'Utilization of synchrotron radiation and drug discovery'. Each symposium included 5 lectures. The lectures 'Forefront studies on carbon nanotubes' (K. Suenaga, AIST), 'Structures of novel nano-materials determined by synchrotron radiation powder experiment' (M. Takata, JASRI/SPring-8), 'Electronic state analysis by the nano scale' (M. Terauchi, Tohoku U.), 'Evaluation of the nanotech device by synchrotron radiation micro-beam diffraction method' (S. Kimura, JASRI/SPring-8), and 'Nano magnetic structure analysis of the manganese system super enormous magnetic resistance material' (S. Mori, Osaka Pref. Univ.) were included in the former symposium. And 'Present state and prospect of the Saga synchrotron radiation facilities' (K. Watanabe, Saga U.), 'The structural biology which aimed at drug discovery' (N. Tanaka, Showa U.), 'The development of the inhibitor considering the metal ion effect of human hematopoietic prostaglandin D synthase' (T. Inoue, Osaka U.), 'Denovo molecular design which makes the three-dimensional protein structure to be a target' (T. Matsuzaki, Mitsubishi Chem. Co.), and 'Development of AIDS medicine: Molecular mechanism of the drug resistance and crystal structure analyses' (H. Mitsuya, Kumamoto U.) were in the latter. The plenary lecture titled 'Superconductivity and magnetic characters of boron/carbon compound' was also carried out by J. Akimitsu (Aoyama-gakuin U.).



Awardees of 2003 Annual Meeting and President of CrSJ: N. Shibata, D. Hashizume, N. Yasuok (President), and T. Hakoshima.

At the annual CrSJ Awards Ceremony, a Research Award was given to T. Hakoshima (Nara Inst. of Sci. & Tech., NAIST); and the Young Crystallographer Awards went to N. Shibata (Himeji Inst. of Tech.) and D. Hashizume (Riken Inst.). The Local Chair was Y. Yamagata (Kumamoto U.) and the Program Chair was S. Ikemizu (Kumamoto U.). Full details of the meeting program can be viewed at CrSJ home page wwwsoc.nii.ac.jp/crsj/index-e.html.

Tsuyoshi Inoue

MEETING REPORT

Electron Crystallography School

Moscow, Russia – June, 2003

Participants of the Electron Crystallography School.

A school on electron crystallography was held in Moscow in June, 2003 at the Inst. of Crystallography of the Russian Academy of Science (ICRAS). The school was organized and supported by the IUCr Commission on Electron Diffraction. The school celebrated the 60th anniversary of the founding of IC RAS where the method of structural analysis using electron diffraction (EDSA) was born and developed. The founders of the EDSA method in Russia were Z. Pinsker and B. Vainshtein, who became the director of the Inst. of Crystallography. A wide range of structures including thin films, metals and alloys, oxides, semi-conductors, catalysts and complex minerals have been studied by electron crystallography in many labs around the world.

The objective of this school was to provide basic instruction for PhD students and scientists interested in applying electron crystallographic techniques in structure studies of inorganic materials and nanostructures. The subjects of the school were: image formation and diffraction, kinematical and dynamical theory; direct methods and maximum entropy in theory and practice for crystal and surface structure determination; data processing in HREM images, crystal structure determination; quantitative CBED and its application to crystal structure determination; precise electron diffractometry for quantitative crystal potential and bonding analysis; electron diffraction on specific samples (texture patterns for minerals, diffraction on gases etc.); CCD cameras and image plates for electron crystallography; and orientation imaging microscopy. Practical training with software and exercises was an essential part of the School.

Experts in the field of electronic crystallography taught the school: L. D. Marks (USA), K. Tsuda (Japan), Hua Jiang (Finland), T. Wierich (Germany), M. Jemmi (Italy), Rene de Kloe (USA). Lecture were also presented by: A. Kiselev, A. Avilov and V. Klechkovskaja (Russia), L. Vilkov (Russia), and M. Nikolsky (Russia).

The majority of the students (80 %) were from Russia. A visit to Moscow's Kremlin made an indelible impression on the participants of the school.

The school would not have been possible without the financial support from the IUCr, the Ministry of Science and Technologies of Russia, Interactive Corp. (JEOL) and EDAX that made it possible to solve many organizational problems and provided financial support to young scientists. The assistance of the former Chairman of the IUCr Commission on Electron Diffraction, D. Dorset, and the organizer of previous schools on electronic crystallography in Europe, Sven Hofmoller, is greatly acknowledged.

Anatoly Avilov

MEETING REPORT

Croatian-Slovenian Crystallographic Meeting

Plitvice Lakes, Croatia, June, 2003



Plitvice Lakes, Croatia

The Twelfth Croatian-Slovenian Crystallographic Meeting was held in National Park Plitvice Lakes, Croatia, June 19–22, 2003. It was jointly organized by the Croatian Crystallographic Assn and the Slovenian Crystallographic Soc. The honorary presidents of the meeting were Boris Kamenar (Zagreb), and Ljubo Golic (Ljubljana).

The plenary lecturers of the meeting were: B. Kojic-Prodic and Z. Stefanic (Zagreb): 'Hydrogen bonding and supramolecular architecture'; G. Vlaic (Trieste): 'XAFS spectroscopies and chemistry: some selected results'; J. P. Abrahams and N. Ban (Zurich): 'X-ray crystallographic structure determination of large asymmetric macromolecular assemblies'; A. Golobic (Ljubljana): 'Solving structural problems of ceramics materials'; A. Danilovski (Zagreb): 'Biological and pharmaceutical solids in the crystallographic arena'. We were pleased that E. Tillmanns (Vienna) and H. Wondratschek (Karlsruhe) participated in the meeting. There were 82 registered participants from 10 countries and 52 contributed abstracts. There were 135 authors on the papers with a high probability that their surname began with the letter P.

The meeting covered a large area of crystallographic science with stress on chemical crystallography and investigations on organic, coordination, small biological and organometallic crystals. We had contributions from physical crystallography, computing, powder diffraction, small angle scattering,

electron microscopy, mineralogy, alloys, films material science and protein crystallography. The most common word of the meeting was 'nano' in many variations: nanocrystalline, nanowire, nanotubes, nanostructure, nanosized particle, nanodevices, nanoribbons and some more. Thanks goes to all the sponsors, because of them this meeting was organized without registration fee for any participants.

The 13th SLO-CRO Crystallographic Meeting will be held in Lipica, Slovenia June 17–20, 2004. For further information contact ivan.leban@uni-lj.si or visit <http://rcul.uni-lj.si/~fn01leban/slkr/>.

S. Popovic (Zagreb) and I. Leban (Ljubljana)

Dear Professor Popovic,

Having returned well to Karlsruhe yesterday evening, I should like to express my sincere thanks to you and to the organizing team for this excellent conference. I enjoyed the interesting lectures (it was the first meeting after several years), the nicely situated and well kept hotel and, last not least, the beautiful surroundings with the many clear lakes, with the numerous waterfalls and its flora and fauna.

I became acquainted with several of your colleagues and students and enjoyed to talk with them and to discuss their and my problems. Now I am 'back in the salt mines' again and found here some mail concerning the new volume of International Tables which brings me to reality. The last week will stay in my memory, and I am looking forward to visiting your next conference, then in Slovenia.

Hans Wondratschek

MEETING REPORT

Applied crystallography

Kraków, Poland, September, 2003

C. Giacobazzo, School Director, giving an interview about the school to the local TV program

The XIX Int'l Conference on Applied Crystallography was held in Kraków, Poland, September 1–4, 2003. As with the previous conferences, this one was organized by the Inst. of Physics and Chemistry of Metals of the U. of Silesia in Katowice. This time the conference was followed by the Summer School on Polycrystalline Structure Determination by Direct Methods (September 4–7, 2003). The Committee of Crystallography and the Committee of Material Science of the Polish Academy of Sciences were the co-organizers of both events. The IUCr awarded scholarships to enable young scientists to attend the conference and the school. The conference was also sponsored by the Rector of the U. of Silesia, Polish Ministry of Nat'l Education and Polish Academy of Sciences.



Conference participants at one of the oral sessions.

One hundred and twenty four participants from 18 countries gathered and engaged in lively discussions throughout the plenary, oral and posters sessions. There were 38 oral and 78 poster presentations. The plenary lectures were given by prominent scientists in the field of crystallography and structural studies - A. Authier, D. Balzar, H.J. Bunge, R. Cernik, J. Fiala, C. Giacobazzo, F. Izumi, P. Klimanek, G. Kostorz, K. Lukasiewicz, P. Scardi, V. Shekhtman and others. Topics included: development of methods and techniques in X-ray studies, crystal structure determination methods, crystallography of phase transformations, texture analysis, material structures – metals and alloys, ceramics, polymers, thin films, quasicrystals, amorphous materials, nanomaterials, and molecular crystals. For example, the traditional methods of line profile analysis have been widely discussed in view of their recent development in the field of powder pattern modelling based on a complex analysis of factors influencing line broadening such as defects, crystallite shape and distribution and others. Special attention was also paid to texture analysis including the problem of the influence of non-uniform dislocation density in hexagonal crystals. Also new programs for crystal structure determination consisting of a combination of direct methods and Montecarlo techniques as well as programs for structure refinement were presented.

The conference proceedings will be published by the World Scientific Publishing Co.

The organizers also took care of the social aspects, including an excursion to the Wieliczka salt mine – one of the oldest salt mines in Europe.



Computer session

The School was organized as the conference satellite meeting. Solving crystal structures from powder data is not only a scientific challenge but also the solution for many industrial and technological problems. Teaching young scientists the expertise and know-how on the methods for crystal structure determination was the main purpose of this school. Under the direction of C. Giacovazzo and tutorship of C. Baerlocher, D. Balzar, E. Cheung, C. Giacovazzo, W. Lasocha, A.J. Markvardsen and P.E. Werner, 46 participants attended the lectures and practiced their skills at the extended computer sessions. The lectures were basic and advanced and covered powder indexing, full pattern decomposition, direct methods for crystal structure determination, Montecarlo methods, Rietveld refinement. Patterson techniques, structure solution from Powder Diffraction Data Using Evolutionary Algorithms. The students became familiar = with the following programs: ITO, DICVOL91, N_TREOR, PIRUM, PFLM, EXTRA, EXPO2002, DASH.

Danuta Stroz, Conference Secretary

MEETING REPORT

High pressure crystallography

Erice, June, 2003

The 34th crystallographic Course at Erice (June 4-15, 2003), a NATO ASI and a EuroSummerSchool, was devoted to high-pressure crystallography. This topic was selected for the first time in the history of the Erice meetings. The Course directors – A. Katrusiak (Adam Mickiewicz U., Poznan, Poland) and P. F. McMillan (U. College, London, UK), and the team guided by P. Spadon (Padova U., Italy) and L. Riva di Sanseverino (Bologna U., Italy) made the course an unforgettable event for all participants – students and lecturers, the 'Erice veterans' and for those, who were in Erice for the first time.

The idea of the course originated from the High-Pressure Commission of the IUCr in 1998. The main objective was to provide crystallographers worldwide with a basic training, which would enable them to apply the 'neglected' thermodynamic parameter of pressure more commonly in their research.



Group photograph of the award ceremony: on the top: P. F. McMillan and A. Katrusiak directors of the course; first row from left to right: L. Riva di Sanseverino, A. Budzianowski, S. Filipek, E. Boldyreva, T. Hirata, P. Spadon, Mrs. Paz-Pasternak, R. Fourme, M. Paz-Pasternak, S. Kazantsev, A. Dewaele, G. D. Gatta.

The program was 'densely packed' and covered all possible branches of high-pressure research: solid state chemistry at high pressure (P. McMillan, E. Boldyreva), the high-pressure crystallography of gas hydrates (W. Kuhs) and amorphous ices (L. Pusztai), equations of state, thermophysical properties of solids under pressure, phase transitions (W. Holzapfel, R. Angel), computational techniques (B. Winkler, J. Tse, M. Parrinello, A. Oganov), experimental techniques (M. Paz-Pasternak, R. Angel, M. McMahon, O. Shimomura, D. Haeusermann, M. Mezouar, L. Dubrovinsky, J.-P. Itie), high-pressure studies of molecular crystals (J. Loveday, A. Katrusiak, E. Boldyreva, M. Szafranski), soft materials and biomaterials under pressure (S. Gruner, R. Fourme), perovskites (F. Rodriguez), cuprate superconductors (A. Gauzzi), metal and metal alloys (M. McMahon, V. Degtyareva), magnetic properties (M. Paz-Pasternak, I. Goncharenko), quasicrystals (G. Krauss), superhard phases (V. Solozhenko), analysis of strain by convergent beam electron diffraction (A. Armigliato), structure maps for constrained structures (J. Parise), 'stuffed' framework structures (N. Ross), solid-state transformations under high dynamic pressures (S. Batsanov), modulated structures (V. Petricek). High-level lectures, numerous tutorials, 10 workshops (some of them repeated), two poster sessions, formal and informal discussions – all this has contributed to a real success of the course not less, than traditional Erice excursions, Marsala, singing and dancing...

The meeting was sponsored and generously financed by the European Commission, DG XII, TMR Programme, EuroSummerSchools, Bruxelles; by the IUCr, Chester; by NATO Scientific Affairs Div., Bruxelles. Support under the form of Awards of Liberal Contributions have been received from B & B HT Moscow, RU; Bruker-Nonius, BV, Delft, NL; D'Anvils Ltd. Kfar-Saba, IL, and Almax Industries, Diksmuide, B.

A representative of the NATO Science Commission, J. Howard, gave an introduction into the various NATO activities supporting research worldwide. The representatives of the B & B HT Moscow, RU, and of the D'Anvils Ltd. Kfar-Saba, IL donated valuable prizes – diamond anvils and a diamond anvil cell – to the selected posters. The 'Erice Vaciago Award' for the most active young participant in the lecture hall went to Sergei Kazantsev (Moscow, RU).

For some of the participants the course will be surely a beginning of the research in a new fascinating field, for others a beginning of new professional contacts, that can well develop into personal friendships (as it often happens to Erice contacts). It is also very important to mention, that this course was the first course in the history of the whole Majorana Centre activity, that was accessible to everyone worldwide via internet 'in real time' (the lecturers even received questions and comments not only from the Erice audience, but also from other countries 'on line'). The course is still accessible to anyone interested in it. The presentations and the videos of the lectures can be downloaded from the site www.crystalerice.org or, more directly, from <http://erice2003.docking.org>. If necessary, J. Irwin (jjj@cgl.ucsf.edu) will surely help with advice and assistance. The course proceedings are being published by Kluwer as the book entitled 'High-Pressure Crystallography', edited by the Course Directors. The course was incredibly open for those, who were unable to attend due to some reason (lack of money, physical disability, limitations on the number of participants in Erice, etc.). The lecturers sincerely tried to bring their knowledge and experience to as large and diverse audience, as possible. One could only wish that this becomes a new tradition of Erice (and not only) courses.

Elena Boldyreva

MEETING REPORT

ISCGTIEM

Mysore, India, January, 2003



The Int'l School on the Crystal Growth of Technologically Important Electronic Materials, organized by K. Byrappa (U. India) and R. Fornari, (Italy), was held in Mysore, India, January 20-28, 2003. The school was supported by the IUCr, the Indian Defence Ministry, CSIR, U. of Mysore and industries and public organizations in Mysore. The school had 90 students and 30 tutors from 20 different countries. The school presented both fundamentals and recent advances in crystal growth and included historical and theoretical concepts and techniques of growing and characterizing crystals.

The ISCGTIEM was opened by the Honorable Union Minister, Govt. of India, V. Srinivasa Prasad. In an inaugural address, K. Lal, (Director, Nat'l Physcial Lab, New Delhi) described the development of crystal growth science in India from the days of A. R. Varma.

R. Fornari, Chairman of the IUCr Commission on Crystal Growth, described the activities of the Commission. H. Klapper (Germany) discussed the history and objectives of IUCr Commission schools. The Honourable Vice Chancellor of the U. of Mysore, K. S. Hegde announced the publication of a comprehensive book on hydrothermal research 'Handbook of Hydrothermal Technology, A Technology for Crystal Growth and Materials Processing' by K. Byrappa (India) and M. Yoshimura (Japan). N. D. Tiwari (Registrar, U. of Mysore), announced the publication of the ISCGTIEM Proceedings Book, edited by K. Byrappa, T. Ohachi, H. Klapper, and R. Fornari and published by Allied Science Publishers, New Delhi.

P. Rudolph (Germany) spoke on stoichiometry-related growth phenomena and discussed the state of the art of industrial scale GdAs crystal growth. F. Abbona (Italy), spoke on crystal growth from solutions, covering solvents, solubility, supersaturation, surface structure, nucleation, growth kinetics and the effect of impurities. In a lecture on heterogeneous nucleation and crystal network formation, X. Y. Liu (Singapore) discussed crystallization kinetics and thermodynamic models. He emphasized the importance of novel technologies in controlling crystallization and pattern formation at low temperatures. Y. Furukawa (Japan), spoke on pattern formation of ice crystals during growth from supercooled water. H. Klapper discussed rapid growth of crystals from solution. The demand for huge KDP crystals of edge length up to 60 cm for laser fusion led to the development of a new method of crystal growth that reduced growth time from 18 months to a few weeks. T. Ohachi discussed the bulk and surface morphology of silver chalcogenides at equilibrium and non-equilibrium conditions in which interface morphology is controlled by the transport species for the growing crystal shape. There were lectures on modelling of crystal growth processes by T. Duffar (France), Q.-S. Chen (China) and J. P. J. M. Van der Eerden (The Netherlands). A. Moreno (Mexico) delivered lectures on the influence of electric and magnetic fields upon protein crystallization. K. Byrappa reviewed the status of the hydrothermal method of growing crystals of rare earth vanadates and quartz.

There were lectures on growth of crystals from melt. R. Fornari covered fundamental concepts, and H. Dabkowska (Canada) discussed the growth of oxide single crystals by the optical floating zone method. A session on crystal growth and characterization of single crystals of SiC (a wide band-gap semiconductor) featured lectures by T. Sudarshan (USA), I. Bhat (USA), G. Dhanaraj (USA) and Q.-S. Chen.

A session on vapour phase growth included lecturers on vapour phase epitaxial growth and properties of nitrides (R. Fornari), MBE growth of high index GaAs and GaN on Si using microwave plasma (T. Ohachi), dislocation reduction in lattice-mismatched heterostructures (Z. R. Zytkeiwicz, Poland); and CVD growth and characterization of ZnS (V. K. Wadhawan, India). H. Strunk (Germany) discussed microepitaxial growth and transmission electron microscopy for defect characterization of semiconductor crystals. D. Bliss (USA), lectured on bulk crystal growth by vertical gradient freezing, and T. Simecek (Czech Rep) described the importance of LPE.

Other lectures concerned crystal growth in microgravity (T. Hibiya, Japan), in space (T. Duffar), in vacuum and beyond (E. Vlieg, The Netherlands). K. Soga (Japan) described the preparation of icosahedral cluster solids and their applications in modern electronics. The character of the icosahedral cluster, an intermediate between semiconductor and metal, is the most favorable one for thermoelectric converters. Similarly, boron-rich icosahedral cluster solids are potential candidates for high T_c superconductors due to their high density of state at the Fermi level.

A cultural evening was organized and the students and faculty of the Fine Arts College of the U. of Mysore entertained ISCGTIEM delegates with Indian folk, classical and traditional dances and music. An excursion to historical sites and national monuments (Belur, Halebeedu and Shravanabelagola) was organized.

The lectures were recorded, a video CD is available, and the proceedings can be obtained from K. Byrappa, byrappak@yahoo.com.

K. Byrappa

NOTICE

Announcing...



In recognition of the growing international and interdisciplinary nature of structural biology, three organizations have formed a collaboration to oversee the newly formed worldwide Protein Data Bank (wwPDB; www.wwpdb.org/). The Research Collaboratory for Structural Bioinformatics (RCSB), the Macromolecular Structure Database (MSD) at the European Bioinformatics Institute (EBI) and the Protein Data Bank Japan (PDBj) at the Institute for Protein Research in Osaka U. will serve as custodians of the wwPDB, with the goal of maintaining a single archive of macromolecular structural data that is freely and publicly available to the global community.

The wwPDB represents a milestone in the evolution of the Protein Data Bank (PDB; www.pdb.org/)^{1,2}, which was established in 1971 at Brookhaven Nat'l Lab as the sole international repository for three-dimensional structure data of biological macromolecules. Since July 1, 1999, the PDB has been managed by three member institutions of the RCSB: Rutgers, The State U. of New Jersey; the San Diego Supercomputer Center at the U. of California, San Diego; and the Center for Advanced Research in Biotechnology of the Nat'l Inst. of Standards and Technology.

The wwPDB recognizes the importance of providing equal access to the database—both in terms of depositing and retrieving data—from different regions of the world. Therefore, the wwPDB members will continue to serve as deposition, data processing, and distribution sites. Deposition procedures will not be altered by the formation of the wwPDB; data can still be deposited using ADIT at the RCSB and PDBj or by using AutoDep at the EBI.

To ensure the consistency of PDB data, all entries will be validated and annotated following a common set of criteria. All processed data will be sent to the RCSB, which distributes the data worldwide. All format documentation will be kept publicly available and the distribution sites will mirror the PDB archive using identical contents and subdirectory structure. However, each member of the wwPDB will be able to develop its own web site, with a unique view of the primary data, providing a variety of tools and resources for the global community.

An Advisory Board consisting of appointees from the wwPDB, the International Union of Crystallography and the International Council on Magnetic Resonance in Biological Systems will provide guidance through annual meetings with the wwPDB consortium. This board is responsible for reviewing and determining policy as well as providing a forum for resolving issues related to the wwPDB. Specific details about the Advisory Board can be found in the wwPDB charter, available on the wwPDB website.

The RCSB is the 'archive keeper' of wwPDB. It has sole write access to the PDB archive and control over directory structure and contents, as well as responsibility for distributing new PDB identifiers to all deposition sites. The PDB archive is a collection of flat files in the legacy PDB file format³ and in the mmCIF4 format that follows the PDB exchange dictionary (<http://deposit.pdb.org/mmcif/>). This dictionary describes the syntax and semantics of PDB data that are processed and exchanged during the process of data annotation. It was designed to provide consistency in data produced in structure laboratories, processed by the wwPDB members and used in bioinformatics applications. The PDB archive does not include the websites, browsers, software and database query engines developed by researchers worldwide.

The members of the wwPDB will jointly agree to any modifications or extensions to the PDB exchange dictionary. As data technology progresses, other data formats (such as XML) and delivery methods may be included in the official PDB archive if all the wwPDB members concur on the alteration. Any new formats will follow the naming and description conventions of the PDB exchange dictionary. In addition, the legacy PDB format would not be modified unless there is a compelling reason for a change. Should such a situation occur, all three wwPDB members would have to agree on the changes and give the structural biology community 90 days advance notice.

The creation of the wwPDB formalizes the international character of the PDB and ensures that the archive remains single and uniform. It provides a mechanism to ensure consistent data for software developers and users worldwide. We hope that this will encourage individual creativity in developing tools for presenting structural data, which could benefit the scientific research community in general.

Acknowledgments

The RCSB PDB is supported by funds from the Nat'l Science Foundation, the Dept. of Energy, and the Nat'l Institutes of Health. The MSD-EBI is supported by funds from the Wellcome Trust, the European Union (TEMBLOR, NMRQUAL, SPINE, AUTOSTRUCT, and IIMS awards), CCP4, the Biotechnology and Biological Sciences Research Council (UK), the Medical Research Council (UK), and the European Molecular Biology Lab. PDBj is supported by grant-in-aid from the Institute for Bioinformatics Research and Development, Japan Science and Technology Corp. (BIRD-JST), and the Ministry of Education, Culture, Sports, Science and Technology (MEXT).

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OBITUARY

Harry Francis West Taylor (1923-2002)



H. F. W. Taylor, energetic, forthright and an enthusiastic supporter of careers for women long before this became PC, was always known as 'Hal' to his colleagues and friends. His scientific career spanned over fifty years and saw great changes in crystallography, from home-made equipment and Beevers-Lipson strips to automatic diffractometers and high-powered computers.

He began his studies at the U. of Nottingham, then Birkbeck College, London (1948 - 1953), which provided a uniquely stimulating environment, in large part due to the presence of the late J. D. Bernal. While there, he worked on a range of topics using methods and equipment that were incredibly primitive by today's standards. He used to recount that his introduction to crystallography commenced by being told by Bernal to build his own film cassette for a single crystal camera from a tin can and bicycle clips.

In 1953, he was offered a permanent post in the Chemistry Dept at Aberdeen U., where he remained until his retirement. On arrival there, his interests turned to mineralogy and the crystal structures of the naturally occurring calcium aluminate and silicate hydrates, especially as a route to elucidating the structures of the poorly-crystallised cement phases. In addition to solving many crystal structures by x-ray crystallography, he quickly realised the potential of electron microscopy and diffraction. With the late J. A. Gard, he solved mineral structures for which only poorly-crystallised or disordered minerals or fine-grained synthetics were available.

Hal became interested in topotactic reactions in various structures, particularly silicates; I was one of his first research students, and was privileged to work with him on this. He was a stimulating supervisor, and during that time we - following the string-and-sealing-wax tradition - built apparatus to do the work and succeeded in studying a number of mineral transitions.

The advent of automatic diffractometers and high-powered computers opened a new world to Hal. No longer was peering at spots on film to gauge their intensity followed by laborious calculations: Hal seized on the advances with gusto, and became an enthusiastic computer programmer.

Hal was an excellent and inspiring supervisor. His enthusiasm for crystallography was unbounded and he gave unstintingly of his time and intellect to others. He regularly attended crystallography meetings, both national and international, and I remember many stimulating discussions arising from these. He served on the committee of the Crystallography Group of the Inst. of Physics (before the days of the BCA!).

Hal also contributed to undergraduate teaching, assuming a full share of lecturing, tutorials and laboratory work.

Hal was a clear and careful writer. He edited a multi-authored two-volume book on cement chemistry, which appeared in 1964. Writing his own book on the subject had to wait until later, but the first edition (1990) and fully revised second edition (1997) have probably become the most widely read single text on cement. The book has been translated into several languages and, moreover, several pirate editions - perhaps the ultimate accolade of a successful science book - were also made!

Hal served a term as head of department, 1977 - 1980, conscientiously but without great enthusiasm; administration held no charms for him, and it was increasingly a time of stringency and retrenchment

within the University. After the completion of a term as head of department, 1977 - 1980, he took partial and later full retirement from Aberdeen, to pursue research and writing. A series of honorary Professorships followed, first at the Imperial College, London and subsequently at Leeds.

Formal retirement meant more time for mountaineering - a lifelong interest that began in Wales and subsequently encompassed all the Scottish mountains and many of the European alpine peaks as well as others in the Americas, Asia and Africa. He remained in excellent physical condition until late in life, when increasing heart trouble forced an operation. He remained professionally active and only succumbed - quite suddenly - while journeying home from a meeting abroad.

Hal's career attracted many honours and distinctions. He was on the editorial boards of numerous journals, and was a Fellow of many organizations including the Royal Society of Edinburgh. He received the Kroll medal and prize of the Inst. of Materials and The Copeland award of the American Ceramic Soc. amongst many distinctions.

We shall remember him for his unbounded enthusiasm and zest for life, his inspiration of students and colleagues, generosity in sharing ideas, and - on a personal level - his wonderful down-to-earth sense of humour. We miss him greatly.

He is survived by his wife, Joan, and a son, Robin, to whom we extend our deepest sympathies.

Lesley Dent Glasser

OBITUARY

Bertram Neville Brockhouse (1918-2003)

Taken from www.physics.mcmaster.ca/people/fs3_people_Brockhouse_BN.html

*The following biography was prepared at the time of his retirement in 1984. It is taken from *Physica 136B* (1986) xxvii-xxxii (North-Holland, Amsterdam)*

Bertram Neville Brockhouse was born July 15, 1918 in Lethbridge, Alberta. After graduating from high school in 1935, he obtained his Ph.D. from the U. of Toronto in 1950, with a thesis entitled 'The Effect of Stress and Temperature upon the Magnetic Properties of Ferromagnetic Materials'.

In July 1950 Brockhouse joined the staff of the Atomic Energy Project of the Nat'l Research Council of Canada at the Chalk River Nuclear Labs, northwest of Ottawa. His work at Chalk River involved studies of the resonant scattering of slow neutrons by strong absorbers such as cadmium and samarium. The measurements were made by placing the sample in a well shielded scattering chamber so that it was surrounded by an annular array of six Bismuth Fluoride detectors. The chamber was mounted on the arm of a single-axis spectrometer which had been built in the late nineteen-forties.

The idea of studying the inelastic scattering of slow neutrons occurred at a meeting Brockhouse attended in December 1950. It was soon decided that such experiments were feasible at the Chalk River reactor which was at the time, the world's highest flux beam reactor. The resonant scattering apparatus was used to study the energy distributions of initially monochromatic neutrons scattered by polycrystalline samples. The intensities of neutrons transmitted through various thicknesses of cadmium were compared with calculations based on ideal gas and Einstein models of the vibrational behaviour of the material.

Early in 1952 Brockhouse put together what he described as a 'large aperture double spectrometer', hoping to be able 'to measure the as yet unknown frequency distribution of normal modes' in a crystal. In 1953 he took advantage of an unexpected shutdown of the NRX reactor to spend ten months as the first foreign guest scientist in the Reactor Dept at Brookhaven National Lab. He worked on multiple scattering by flat specimens, magnetic scattering by zinc ferrite, powder magnetic diffraction studies of copper oxide, the development of improved monochromator crystals, and measurement of the incoherent cross sections of copper and gold.

On his return to Chalk River, Brockhouse again set up his crude triple-axis spectrometer, using a fixed angle monochromator facility with an aluminum crystal monochromator, a makeshift sample table, with the old single-axis instrument acting as the analysing spectrometer. The scattering angle at the sample position was fixed for a given set of measurements but could be changed by turning the sample table and moving the analysing spectrometer. The machine was used successfully for studies of the phonon frequency distribution of vanadium and the inelastic scattering by liquid lead and heavy water.

In the early months of 1955, 'preliminary measurements were made of energy distributions scattered by an aluminum single crystal in several different orientations'. This work led to the first successful determination of a phonon dispersion curve. It provided the first convincing demonstration of the power of the triple-axis method, at a time when groups at Saclay and Brookhaven were concentrating on a complementary time-of-flight technique.

Brockhouse next turned his attention to the possibility that neutrons might be used to investigate the 'thermal disturbances of the magnetized arrays of...coupled magnetic moments (which) can be described by means of quantized wave excitations called spin waves'. The ferrimagnetic material magnetite was chosen because large single crystals were available. The measurements of scattered neutron energy were carried out for 12 different orientations of the crystal, and it was concluded that the observed excitations were not phonons, but indeed 'in the spin system itself'. This was the first experimental determination of a magnon dispersion curve. These experiments were followed by extensive sets of measurements on a variety of crystals.

By the mid-fifties Brockhouse had begun to put together a beryllium filter-chopper spectrometer. The instrument was similar to the slow chopper at Brookhaven except that a filter difference technique was used to improve the overall energy resolution. Phonons in aluminum and beryllium were studied using the filter-chopper spectrometer, and an important series of measurements on water was completed.

A new type of high resolution time-of-flight instrument was devised by Brockhouse at about this time. This was the rotating crystal spectrometer, first mentioned in an AECL Physics Div. progress report in late 1957. This machine was installed at the NRX reactor, and an improved version, fitted with a cooled quartz filter, was later set up at the N5 hole of the new reactor NRU (Nat'l Research Universal).

The famous C5 triple-axis spectrometer, immortalised in Kittel's 'Introduction to Solid State Physics', was installed at the NRU reactor in 1958. This machine was an important training ground for many present day triple-axis spectrometrists. The first material to be studied using the C5 machine was a single crystal of silicon. Major improvements to the spectrometer were reported in 1959, including the construction of monochromating crystal control units with which 'it was possible to change the wavelength of the incoming neutrons automatically and continuously over a wide range'.

With the capability to vary the incident neutron energy of the C5 spectrometer, a new method for the study of high energy excitations became possible. This was the beryllium filter detector method, first tried at Chalk River in early 1960. Soon the N5 rotating crystal spectrometer was modified so that both the incident energy and the angle of scattering could be continuously varied.

During his highly productive years at Chalk River Brockhouse found time to take part in three Gilbert and Sullivan operettas, and a production of Shaw's 'Arms and the Man'. In 1962 Brockhouse moved to McMaster U. where remained until his retirement in 1984. At McMaster he took an active part in teaching, and was able to communicate his enthusiasm for physics to undergraduate and graduate students alike. He was influential in building up the department, and he and his graduate students built new spectrometers at the McMaster Nuclear Reactor, and later at the Chalk River NRU reactor.

Prof. Brockhouse received many honours over the years, including the Tory Medal of the Royal Society of Canada, the Buckley Prize of the American Physical Society, the Duddell Medal and Prize of the (British) Inst. of Physics and Physical Society 'for excellence in experimental physics', and the Centennial Medal of Canada. He received the Nobel Prize in 1994 for designing the Triple-Axis Neutron Spectroscopy and his use of it to investigate Condensed Matter.

We owe a tremendous debt of gratitude to Bert Brockhouse. He has inspired many people to accept the challenges of neutron inelastic scattering, and to work long and hard to improve methods, materials and equipment in order to be able to do experiments properly and convincingly. Throughout his career he has demonstrated an honesty, thoroughness and scientific passion which are an example to us all. The 'absent-minded professor' stories are plentiful, and amusing, but the stories of his insistence on good experimental technique, and of his concern that time and money be efficiently used, are perhaps more to the point. His intuition, his dedication to research, and his kindness and concern for his fellow workers, are frequently mentioned by those who have had the pleasure to work with him.

John R.D. Copley, McMaster Nuclear Reactor, McMaster U., Canada

Footnote: Quotations in the text are taken from published papers and from progress reports of the National Research Council of Canada, Atomic Energy Project, and of Atomic Energy of Canada Limited, Chalk River Project. I am grateful to the many people who contributed information for this brief biography.

NOTICE

Reviewing proposals for NSF grants

The Div. of Chemistry of the US National Science Foundation (NSF) is increasing its pool of reviewers and has asked that chemists worldwide be informed that well-qualified reviewers for its grant applications are needed.

The NSF, which supports basic research and education in science and engineering, recognizes the importance of international participation in its activities. According to A.B. Ellis, director of the NSF Div. of Chemistry Proposals, proposals submitted for funding by US chemists are judged through peer review by respected scientists from around the world who work in academia, government, or industry. Ellis added, 'This enables us to obtain broad, global perspectives on the supported research. In addition, reviewers are occasionally asked to serve on panels and to participate in workshops on emerging research and education themes. The NSF provides support for travel and lodging associated with such activities for all participants. Reviewers benefit from an expanded network of international ties and the opportunity to develop new partnerships related to research, education, and workforce development.'

Interested scientists who have not previously served as NSF reviewers should visit the NSF Web site at www.nsf.gov/mps/divisions/che/news/reviewerinfo.htm. Ellis pointed out that NSF reserves the right to choose reviewers. While they are unable to assure individuals that they will be asked to review proposals, they do attempt to call upon as many qualified reviewers as possible, and they try to limit the number of requests that they make to any single individual, recognizing the many demands reviewers have on their time.

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AWARDS AND PRIZES

Ewald Prize - call for nominations



Professor Michael M. Woolfson (left; Physics Department, University of York, UK) receiving the sixth Ewald Prize from Professors Michiyoshi Tanaka (centre) and Henk Schenk, then IUCr Vice-President and President, respectively, at the opening ceremony of the XIX IUCr Congress in Geneva, Switzerland, on 6 August 2002.

The seventh Ewald Prize, for which nominations are now being invited, will be presented at the XX IUCr Congress in Florence, Italy, in August 2005.

Scientists who have made contributions of exceptional distinction to the science of crystallography are eligible for the Ewald Prize, irrespective of nationality, age or experience. The Selection Committee will give careful attention to the nominations of outstanding scientists who have not yet won a Nobel Prize. Either an exceptionally distinguished scientific career or a major scientific accomplishment may be recognized. Current members of the Selection Committee (see below) and the President of the IUCr are not eligible. No restrictions are placed on the time or the means of publication of the nominee's contributions. The Prize may be shared by more than one contributor, but not more than three, to the same scientific achievement.

Nominations should be submitted to the Executive Secretary, IUCr Secretariat, 2 Abbey Square, Chester CH1 2HU, UK, using the Ewald Prize Nomination Form. **The closing date for nominations is 31 August 2004.** For full details and a nomination form see <http://www.iucr.org/iucr-top/iucr/invitation05.html>

2005 Ewald Prize Selection Committee

M. Tanaka (Japan) (Chair)
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AWARDS AND PRIZES

European crystallography prize



The European Crystallographic Assn (ECA) invites nominations for the fourth European Crystallography Prize to recognize a significant achievement or discovery in crystallography in the past 5-10 years. Nominees should be affiliated or identified with the European crystallographic community, as broadly defined in the charter of the ECA (www.ecanews.org)

The prize, including a monetary award and certificate of recognition, will be awarded at the opening ceremony of the 22st European Crystallography Meeting (ECM-22) in Budapest, Hungary, August 26-31, 2004. Previous laureates are: 2000, Ada Yonath (Israel); 2001, Jochen R. Schneider (Germany); 2003: Carmelo Giacovazzo (Italy).

Nominations should include a statement of the contribution for which the prize is to be awarded and a short curriculum vitae of the nominee. Send postmarked no later than February 28, 2004 to: A. Liljas, Molecular Biophysics, Center for Chemistry and Chemical Engineering, Lund U., Box 124, SE-221 00 Lund, Sweden; Tel: 46 46 222 46 81; Fax: 46-46-222 46 92; e-mail: anders.liljas@mbfys.lu.se

IUCR ACTIVITIES

Single registration system for IUCr online services

The IUCr has brought several of its online services for users, including the World Directory of Crystallographers (WDC) and e-mail alerting for IUCr journals, under a new simple single registration system at <http://www.iucr.org/iucr-top/user/index.html>. In the future, other services such as online submission and review for IUCr journals and subscription to IUCr mailing lists and discussion forums will also be accessible via this system. Each user needs to register information such as their name and e-mail address only once (whether they use all, or only some, of the above services), and can simply and easily keep their own information up to date.

Every registered user is given a unique identifier (their IUCr ID), which can for instance, be optionally included in articles submitted to all IUCr journals. In future, this may, for example, allow a permanent link to be maintained between an article published online and the up-to-date contact and biographical information for each of its authors that exists in the WDC.

Please note: readers who were in the 10th edition of the WDC but have not checked their entry are urged to log in at the above address using their IUCr ID and password. Please direct any queries to wdc@iucr.org.

IUCR ACTIVITIES

Open access and Crystallography Journals Online

There is an increasing trend in scientific journal publishing towards open access, a system of distribution of information where no charge is made to the reader. Making research results freely available has a number of advantages including higher visibility of publications, higher citation rates of open-access publications and access to literature for scientists in the developing world.

The IUCr Executive Committee has therefore decided that from 2004, authors publishing papers in IUCr journals should be given the opportunity to make their papers open access on Crystallography Journals Online. Details are provided at the proof stage. Although a charge is levied for making an article open access, authors unwilling or unable to choose this option are in no way excluded from publishing in IUCr journals as these will contain a mix of both standard and open-access papers.

The charge for making an article open access is USD800. This charge is based on the average cost for the IUCr to produce the first copy of the article, including printing and distribution costs, and includes a contribution to the cost of the long-term preservation and access of the publication. Funds generated from open-access payments will be used to keep subscriptions as low as possible.

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