

INTERNATIONAL UNION OF CRYSTALLOGRAPHY

IUCr Newsletter

Volume 8 · Issue 3

Collected archival edition

Original article text and available illustrations

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LETTER FROM THE PRESIDENT

Letter from the President



Thank you for the enthusiastic emails in response to my last letter. More than 10 offers for translations in different languages and suggestions for the future children's website were received. Continued input will be greatly appreciated!

The Executive Committee (EC) held its yearly three days of intensive meetings in Nancy, France - including a full day devoted to the journals. Important actions taken included: the closure of full-text access to Crystallography Journals Online to non-subscribers, the launch of a new electronic-only journal, the introduction of a Journals Grant Fund (JGF), and the Africa Initiative.

It was always our plan to make the full functionality of the Online site available to subscribers only, with partial functionality available to others. From September 2000 summaries of articles are free, but viewing and downloading articles is restricted to subscribers. Full information and registration procedures may be found at the journals web site (<http://journals.iucr.org>).

The new electronic-only journal, Acta Crystallographica Section E (Structure Reports Online), will be starting in January 2001 and manuscripts are being accepted. Notes for Authors are available at the web site. Subscribers to Acta C will receive Acta E free; Acta E will also have a new subscriber category by which contributors to the journal will be eligible for a reduced subscription rate. Another step into the electronic future!

The Executive Committee is concerned that institutions in many countries, including some within our group of Adhering Bodies, are unable to subscribe to our Journals for economic reasons. To help these institutions keep up with crystallography, we have established a Journals Grant Fund (JGF). Institutions from countries with economic problems may apply for a grant towards part of the subscription costs for each of our Journals. A Sub-committee of the EC will then rank the applications and make recommendations to the EC. Annually, 20 three-year grants will be awarded. In 2001 we will start with 20 one-year grants, 20 two-year grants and 20 three-year grants. More details may be found on the IUCr web site (<http://www.iucr.org>).

Another exciting item on the EC agenda was our Africa Initiative (AI). When Jan Boeyens joined the EC in 1996 he proposed that a crystallographic network be set up in the southern part of Africa. In the past triennium Jan has established an Affiliated Centre for the use of the Cambridge Structural Database in Africa, sponsored by the Cambridge Crystallographic Data Centre (CCDC), the South African National Science Foundation (NSF) and the IUCr. Groups from all over Africa have free access to the database through the Centre. Another achievement was the UNESCO-sponsored transfer of a single-crystal diffractometer from the CCDC to Nairobi, where it is now in operation. In Nancy, the EC decided to sponsor two PhD positions for students from countries in Southern Africa to study for a PhD in South Africa. When they return to their home countries this will strengthen the AI further. Jan and I found much enthusiasm for this programme. Likely co-sponsors include the NSF, South African industries, the CCDC, the International Council for Science, and other charities. The PhD programme may eventually comprise

six to ten positions! In Nancy we described our AI at an ad-hoc meeting with representatives from Bruker, Nonius, Philips and Rigaku who shared our enthusiasm. It may be possible to ship used instruments to places in Africa with arrangements similar to those that accompanied a Nairobi installation. The manufacturers know where good equipment awaits a second life. PhDs in the AI training programme may well return home to well equipped crystallographic laboratories. Our AI is really gaining momentum!

Hendrick Schenk

hs@crys.chem.uva.nl

EDITORIAL

Editorial



This issue includes a long overdue article concerning Dorothy Hodgkin's life and career.

Over a year ago, John Robertson wrote expressing concern that no obituary for Dorothy had ever appeared in the IUCr Newsletter. John agreed to correct the oversight by writing a tribute to Dorothy. Because the wonderful biography of Hodgkin by Georgina Ferry was about to be given wider circulation by a US distributor, Cold Spring Harbour Laboratory Press, it seemed appropriate for John to develop his tribute around a review of the book.

I have been collecting items in the scientific press on women in science and crystallography for years, entertaining the thought of a cover story on the topic. This seemed an opportune time to down load some of that file. (See page 20)

The American Institute of Physics is concerned about under representation by women in physics. Statistical analysis of the membership of the seven scientific societies that make up the AIP, reveals that the American Crystallographic Association has the highest percentage of women members. Women such as Kathleen Lonsdale, Carolyn MacGillavry, Dorothy Hodgkin, Elizabeth Wood, and Gabrielle Donnay in the early days of crystallography, probably have a lot to do with those statistics, but the fact that six of the last thirteen presidents of the ACA have been women is probably an even greater incentive for women to be active in a field where they can influence its direction. It is a pleasure to note the recent election of Fujiko Iwasaki, the first woman president of the Crystallographic Society of Japan.

The cover illustration includes a photo taken at the opening ceremony of the European Crystallographic Meeting in Nancy, where the first European Crystallography Prize was awarded to Ada Yonath of the Weizmann Inst. of Science in Israel in recognition of her pioneering achievements in the crystallographic structure determination and analysis of ribosomes. No one has worked more diligently and tirelessly to determine the structure of the ribosome than Ada. Had it not been for her tenacity at a time when other investigators waxed and waned in their pursuit of the problem, it is unlikely that the recent explosion of extraordinary structural detail on this most fundamental of problems would have occurred.

The large number of scientists who have made critically important contributions to unravelling problems as complex as the structure of the ribosome makes the awarding of prizes extremely difficult. The awarding of a prize provides an opportunity to honor the scientists responsible for an important discovery and to draw the attention of the general public to the significance of the scientific endeavors. It is all too easy to fail to acknowledge properly all individuals whose efforts were critically important to the accomplishment being honored.

Because a problem as large, significant, and complex as the determination of the structure and function of the ribosome requires vital input from numerous investigators, it may be necessary to review the criteria that have traditionally governed nomination and award processes. It has become increasingly difficult to assign credit for a major scientific advance worthy of the Nobel Prize to three individuals. In

fact, the restriction of a scientific award to a limited number of individuals can actually be counterproductive because it may engender hostility and resentment in individuals who have devoted themselves to problems to which they have made a significant contribution and discourage others from engaging in pursuits that are immersed in an atmosphere of intense competition to win, place or show.

LETTER TO THE EDITOR

Reports greatly exaggerated

Dear Bill

Concerning the mistaken report of Waser's death: many years ago, my uncle Julio Bernal (who lived with us at my parent's house) was reported to have died in an air crash. The report was incorrect.

Since he was a very well-liked person, people started arriving at the house in funeral regalia to give us their condolences. After a while, my mother and my uncle got fed up with having to explain and provide refreshments. So, my uncle took a comfortable chair and sat at the porch sipping coffee. It was remarkable the number of cars that slowed down to enter our drive and, suddenly, accelerated away.

Ivan Bernal, Houston, TX

LETTER TO THE EDITOR

Collaboration sought

Dear Bill

I am studying metal-coordination properties of bioactive N,S-donor ligands. I have solved the crystal structure of 4,6-dimethylpyrimidine-2-thiol which acts as a bidentate and a tridentate donor. I wish to pursue computer modeling and SAR studies of the interaction of this and related compounds with biologically relevant receptors. I am seeking a collaborator with expertise in computational chemistry and computer modelling.

Asish Kumar Das
West Bengal, India

LETTER TO THE EDITOR

Metals database

Dear Dr. Duax

I notice in the IUCr Newsletter Vol. 8, No. 2 a paragraph concerning 'Metals in the PDF'. Besides the data bases cited in the article, the most specific collection of data on metallic substances (metals and intermetallic compounds) is CRYSTMET, distributed on CD by John Rodgers (rodgers@snd.cisti.nrc.ca) at a reasonable price for academics. This data base is a valuable tool for people working in the field and among other facilities it contains in graphical form the powder pattern of each compound. For many years, I have been an enthusiastic user and I recommend it to everyone interested in intermetallics.

Maria L. Fornasini
Genova Italy

LETTER TO THE EDITOR

Book donation

Dear Dr. Duax

We are working in crystallography (small molecule structure determination and development of molecular replacement methodology) at the U. of Oviedo, Spain.

We read in the Newsletter that Bill and Kirsten Streib are willing to give away some x-ray crystallography books including books by Buerger. We would be very pleased to obtain any of Buerger's books, which are difficult to find in Spain. The implementation of Buerger's Image Seeking Functions in Macromolecular Crystallography is the subject of our theses.

C. Alvarez-Rua and J. Borge
Oviedo, Spain

Dear Bill

I understand from the second issue (2000) of the Newsletter that Kristen Streib has some journals and basic X-ray crystallography books and wants to give them away. I am the Head of Dept of Chemistry in Kafkas U. which is a recently established University in the East of Turkey. We need such journals and books and would be very pleased to receive them.

Hacali Necefoglu
Kafkas, Turkey

Dear Dr. Necefoglu

Unfortunately, another crystallographer has already secured agreement from a university to cover the cost of shipping the Streib collection to Jordan. I hope that other crystallographers who have Acta collections that need a home will take note of your needs at Kafkas U in Turkey.

Bill

LETTER TO THE EDITOR

Copyright

Dear Bill

I wrote an experiment for our intro chem lab to introduce crystallographic concepts and diffraction. I wanted to use Escher patterns from Caroline MacGillavry's 1965 IUCr publication to show unit cell and symmetry concepts. I asked library personnel to contact the publisher about copyright concerning duplication from a reprint of this volume by Harry N. Abrams, Inc., New York, 1976 with an altered title. After we had printed our manual with photoreduced images of the two figures, we got a response from Abrams saying that we had permission and that we should pay them \$.50 for each copy of each of the two plates. We paid the fee, but I thought it outrageous since Abrams is asking our students to pay for something that they copied from the IUCr. I'm happy to cite them, and I suspect that in the long run that would be a nice advertisement for their book (if it's still in print?).

I am planning to submit a manuscript to the Journal of Chemical Education about this experiment and might like to use these figures there too. They are really only an aesthetic complement to the experiment and unless some better solution can be found, I'll just delete them and substitute something else. Do you have any suggestions on what I should do? I assume that this kind of issue has arisen before this.

Many thanks for any help you can give.

Jim Loehlin
Wellesley, MA
Dear Jim

I have brought your letter to the attention of the Executive Committee of the IUCr. They plan to look into the question of copyright. Meanwhile, you may want to consider generating your own illustrations using packing patterns from real structures, or see the letter below.

Bill

LETTER TO THE EDITOR

Tile designs

Dear Bill

Having taught crystallography, I realize that there are few examples of tilings and nets which can be used to introduce beginners to symmetry. Some teachers use wallpaper patterns, or Escher's artistic symmetrical interlocking animal shapes. Perhaps readers of the IUCr might be interested to find a new book of tile designs which are derived from crystal structures. Geometric Floor Tile Design, Do-it-yourself custom patterned flooring, is aimed at the average home or business owner who wants to create a special interior space. There are detailed practical instructions for design, job planning and installation.

David K. Teertstra
www.tilebooks.com

LETTER TO THE EDITOR

Observing electron density

A reply to Spackman, Howard and Destro

I am grateful to Spackman *et al* for their spirited response (*IUCr Newsletter*, Vol 8, 1, 2000) to my *Nature* News and Views article (*Nature* **401**, 21, 1999) which commented on the work by Zuo *et al* (*Nature* **401**, 49, 1999) and for this opportunity to clarify the situation.

Zuo *et al* used a combination of electron diffraction (to measure low order diffracted intensities) and x-ray diffraction (for higher orders) to determine the charge density in the inorganic material Cu_2O , and my *Nature* News and Views article commented on this work and on the potential application of the combined electron and x-ray diffraction techniques (as suggested in ref 1) to determine the charge density in cuprate superconductors, also inorganic materials of course. The whole thrust of my article was therefore about inorganic materials and for these materials I totally stand by my statement that x-ray diffraction 'is normally unable to give details about the shape of the charge distribution, in particular the shape of the bonds'. I also stand by the reason I gave for this, that the x-ray scattering from dislocations and defects in inorganic materials is normally 'greater than the scattering from the bonding electrons'. It is of interest to note that despite a considerable amount of x-ray diffraction work on cuprate superconductors, which has revealed the atomic positions in these materials, there has been no x-ray determination of charge densities in any cuprate superconductor despite the intense interest in knowing this. If the remarks of Spackman *et al* were correct, that 'extraction of detailed electron density distributions of organic, organometallic, inorganic, ionic metallic and mineral crystalline systems from x-ray diffraction data is now a mature and highly productive field' then surely x-ray diffraction would have determined the charge density in at least one cuprate superconductor by now! The situation is that although x-ray diffraction is a superb technique for determining electron densities in organic, etc., crystals, that is not yet the case for most inorganic crystals. Why is this?

In inorganic materials, the dislocation density is usually at least 10^6cm^{-2} and this can cause x-ray measurements of low order atomic scattering factors to be in error by at least 100%. Accurate measurements of low order scattering factors are essential for determining charge densities since it is the low order reflections which are most sensitive to the degree of ionicity of atoms. Despite the statement of Spackman *et al*, the true situation is that no totally successful scheme for correcting x-ray diffracted intensities has yet been devised for crystals with moderate to high densities of dislocations. Hence x-ray diffraction is normally unable to give details of the charge density for inorganic materials. For electron diffraction, on the other hand, an electron beam focussed to only 1 nm across can be used to select regions of relatively strain free perfect crystal between dislocations in a wide variety of inorganic materials and accurate low order scattering factors *can* be measured by interpreting diffracted intensities using the dynamical theory of electron diffraction. The only inorganic crystals for which x-ray diffraction can be used to give accurate charge densities are crystals which can be grown, or occur in nature, with very low dislocation densities, for example silicon and diamond.

However, although Spackman *et al* are in error concerning most inorganic materials, I gladly agree that for most organic and molecular crystals, x-ray diffraction is a superb technique for measuring charge densities. Why are inorganic and organic materials so different as regards x-ray diffraction measurements of charge densities? The answer lies in the defects. Organic and molecular crystals normally have much larger unit cells than inorganic crystals, and hence dislocations in these materials have much larger Burgers vectors, b , than in inorganic crystals. Since the energy of a dislocation is proportional to b^2 , dislocations have a very high energy in organic and molecular crystals, hence they are energetically unfavourable and the dislocation density in these materials is normally many orders of magnitude lower than for inorganic crystals. Thus x-ray diffraction is an excellent technique for measuring charge distributions in organic and molecular crystals, but for most inorganic materials, the

low order reflections (which are the most sensitive to the ionicities of the atoms) are best measured using electron diffraction.

Colin J Humphreys, FEng
Goldsmiths Prof. of Materials Science

References

1. D. J. Smart and C. J. Humphreys, The application of electron diffraction to determining bonding charge densities in crystals. *Inst. Phys. Conf. Ser.* **52**, 211- 214, 1980.

Dear Bill

Thank you for providing us the opportunity to comment on Humphreys' response to our letter (IUCr Newsletter 8, 2, 2000). We are disinclined to enter into a prolonged scientific argument on this matter, and believe that the substance of the points raised in his response, some of which seem most peculiar to us, will be best judged by the readers.

However, two points deserve emphasis:

- Humphreys mocks our viewpoint thus: 'If the remarks of Spackman et al. were correct, that "extraction of detailed electron density distributions of organic, organometallic, inorganic, ionic, metallic and mineral crystalline systems from x-ray diffraction data is now a mature and highly productive field", then surely x-ray diffraction would have determined the charge density in at least one cuprate superconductor by now!'. Our letter cited two review articles which comprehensively summarized the experimental charge density work for the period 1992 - 1997, listing published x-ray diffraction results on almost one hundred different inorganic materials. Included were studies on several cuprate superconductors and related materials.
- A detailed scientific critique on the original Nature article and commentary has been published: 'On Closed-Shell Interactions, Polar Covalences, d Shell Holes, and Direct Images of Orbitals: The Case of Cuprite', S.-G. Wang & W.H.E. Schwarz, *Angew. Chem. Int. Ed.* 2000, **39**, 1757-1762.

M.A. Spackman, R. Destro and J.A.K. Howard

Dear Bill

In a recent letter to the *IUCr Newsletter* (Vol. **8**, 1, 2000) Spackman, Howard and Destro made a welcome rebuttal of the statement that 'X-ray diffraction is normally unable to give details about the shape of the charge distribution' (*Nature* 401, **21**; 1999). The comments published in *Nature* state that 'while electron diffraction can image electrons, X-ray diffraction is inherently incapable of doing so, as X-rays are scattered by defects in crystals'. Unfortunately, *Nature* did not permit a rebuttal of the statements made, and ignored the Spackman *et al.* letter as well as others, including one by me, sent in response to what appeared in print.

Quite apart from the nature of X-ray scattering (doesn't the widely used kinematic theory assume an imperfect crystal? Isn't extinction, which is the likely cause of the inaccuracy of the low-order X-ray structure factors for the crystals discussed, a result of the crystal being too close to perfect?), and whether or not Cu-Cu bonding has been observed in cuprite, the dramatic announcement '*Orbitals observed*' on the cover of the issue of *Nature* (September 2, 1999) is astonishing, to say the least.

Fortunately, there are now several excellent publications that give hope that Science is still self-correcting. To paraphrase Wang and Schwartz in their comment in *Angewandte Chemie*, in nature (though not in *Nature*), orbitals are mathematical concepts that are not uniquely defined. In a definitive

in-depth analysis (*Angew. Chemie, Int. Edition*, 2000, **39**, 1757-1762,), they point out that although a shift in electron density may appear to have the same features as a text book orbital, the density corresponding to such an orbital is everywhere positive in three-dimensional space, and does not have negative and positive regions.

The *Nature* issue and resulting comments in journals such as *Scientific American* (see for example www.sciam.com/explorations/1999/092099cuprite/index.html) and *Chemical & Engineering News* (1999, **77**, 38), raise the danger that such misconceptions will pervade the teaching curriculum. This issue is addressed most effectively in a timely article by Scerri entitled 'Have Orbitals Really Been Observed?', to appear this fall in the *Journal of Chemical Education*. Scerri notes that 'it is essential that claims of having arrived at a new understanding of such a crucial concept should be subjected to close scrutiny'. The issue has again demonstrated how important it is that the IUCr maintain its own Newsletter. The current tendency for dramatic publicity can only be counteracted when more restrained media are available for open discussion.

Philip Coppens

Buffalo, NY, September 2000

Towards high throughput and dealing with awkward cases:

A snapshot of recent crystallization articles in *Acta Cryst. D*

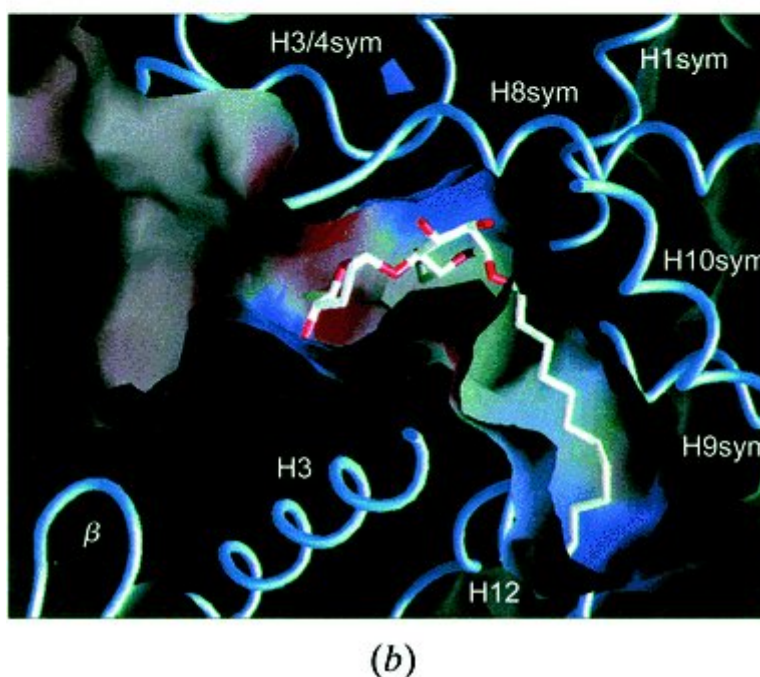
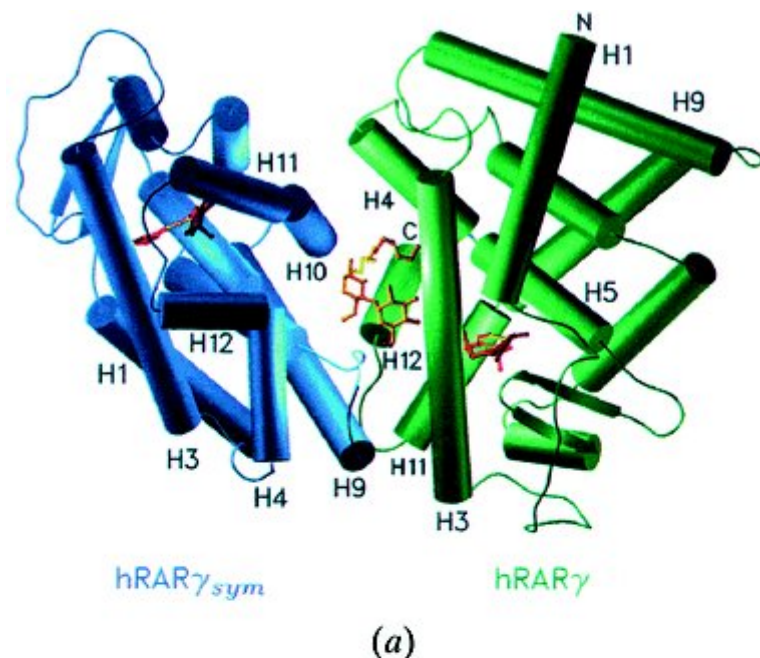


Fig. 1. (a) The dodecyl- α -D-maltoside molecule (in yellow) mediating a crystal contact between two molecules of the hRAR γ LBD/CD564 complex (space group $P4_12_12$; symmetry operators $x - [1/2]$, $-y + [3/2]$, $-z + [3/4]$). The retinoid CD564 is shown in red. (b) GRASP representation of the cavity. 83% of the detergent molecule surface are buried within the crystal contact.

The past years have seen many advances in our ability to solve macromolecular structures and have considerably shortened the time to go from crystal to publication. Cryogenic techniques and more powerful beamlines have resulted in structures often being obtained from single crystals one or more

orders of magnitude smaller than practical a few years ago. The success of the human genome sequencing project highlights the need for new methods for high throughput crystallization and structure determinations. One can imagine that the growth in this field will result in thousands of structures being published in a form similar to small-molecule papers rather than first announcing the crystallization conditions and subsequently publishing the structure and the coordinates. Increased demand has turned the attention of many researchers to crystallization, the main bottleneck to structure determination, i.e. finding conditions to get any crystals and optimization of conditions to turn microcrystals into usable crystals. Crystallization is a multidisciplinary science encompassing biology, chemistry, physics and computing. Embarking on the crystallization of a new protein, one is faced with the choice of where to begin the trial-and-error process. In the past this was guided by previous experience from the purification process, which indicated conditions where the protein is most stable and soluble, likely precipitants, etc., and included one's previous experience with other proteins. To some extent this historical culture has been supplanted by the introduction of rational screening kits. Here, the collected published wisdom has been distilled into a collection of the best recipes of the past. The kits are proving very successful, leading to a boom in crystals from all corners of the living world, from plant, insect, animal or human sources, but the results still rely on trial and error. Even when the screens do not produce crystals they can provide information on solubility useful to the design of conditions suitable for crystallization as in the case of insect neurotoxins from scorpions reported by Guan and co-workers [*Acta Cryst.* **D56** (2000), 1012-1014]. Screening kits have been systematically expanded to include crystallization cocktails that are optimized for different types of macromolecules. Hennessy and co-workers [*Acta Cryst.* **D56** (2000), 817-827] have taken the next logical step. They have mined the Biological Macromolecular Crystallization Database (BMCD), first dividing the macromolecules into hierarchical classes based upon their function and type, and then looking for similarity in the crystallization conditions for each class. A statistical analysis of their database showed significant correlation between the families and conditions employed. This is particularly fascinating, given the potential for variation in protein structure and the fact that even relatively modest modifications, proteolytic clipping, genetic mutations, etc., can determine whether or not one obtains crystals. This procedure has been incorporated into software, which can be used to track ongoing crystallization experiments and extend a laboratory's database. The input data for a macromolecule can include information on its biochemical properties, amino acid composition, solubility, α -helix and β -sheet content determined by circular dichroism and secondary and tertiary structure predicted by various algorithms.

One possible difficulty with the approach of Hennessy *et al.* is addressed in a paper on the crystallization of the matrix protein from Ebola virus [Dessen *et al.*, *Acta Cryst.* **D56** (2000), 758-760]. This protein lacks primary and secondary structural similarity with other known viral matrix proteins, i.e. it has functional but not structural similarity. According to the Hennessy approach, the functional requirements would lead to some similarity in structure, thereby giving a similarity in crystallization behavior. The convergence of the structural and functional similarity is presumably the reason why the hierarchical classification and crystallization approach works. However, other data may be able to correct a strictly functionally based approach. In the case of the Ebola protein, secondary-structure prediction analysis suggests a high β -sheet content, in contrast with the highly α -helical structures of matrix proteins from retroviruses [Conte & Matthews, *Virology* **5** (1998), 191-198] and influenza virus [Sha & Luo, *Nature Struct. Biol.* **4** (1997), 239-244]. When a primary sequence is known, structural inferences based upon it can influence the initial crystallization trials.

One can readily imagine that in the future, groups of laboratories would be able to combine their databases, or add their databases to a central collection, to create a crystallization superdatabase. One problem of the existing BMCD is that it reports only the conditions that gave the best crystals. Marginal crystallization conditions and failures are not reported. It is obvious that knowing where not to look can also be important for obtaining crystals.

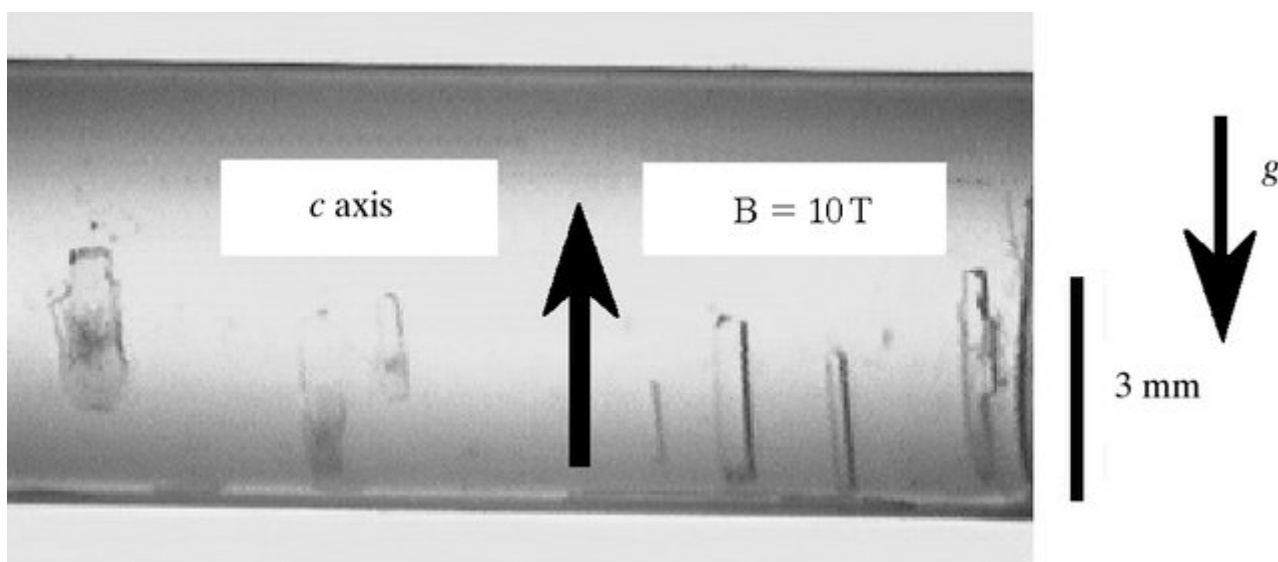


Fig. 2. Orthorhombic lysozyme crystals grown in a magnetic field of 10 T.

Membrane proteins, as a class, are among the most reluctant to crystallize. The use of detergents was a significant breakthrough but has not produced a major increase in the number of membrane protein structure determinations. By binding amphiphilic detergents to the hydrophobic domains these proteins can be made more hydrophilic, and hopefully crystallizable by more conventional methods. Cubic phases are now taking center stage as an alternative approach in membrane protein crystallization [Chiu *et al.*, *Acta Cryst. D* **56** (2000), 781-784]. Rather than mask the hydrophobic part of the protein, these authors make the environment more hydrophobic with a lipid matrix. Use of this technique requires an understanding of the lipid phase diagram, particularly with respect to the detergents used to solubilize the protein. Once the lipid phase behavior was understood, the authors could use a single lipid, monoolein, as a crystallization matrix for several test membrane proteins (two photosynthetic reaction centers, a lightharvesting complex, halorhodopsin and bacteriorhodopsin). Cubic phases do not replace detergents, which are often needed to maintain the molecule in a soluble form prior to crystallization. Non-membrane proteins that have extensive hydrophobic regions may also benefit from detergent use, as in the case reported by Klaholz & Moras [*Acta Cryst. D* **56** (2000), 933-935], where a single dodecyl- α -D-maltoside molecule was found to occupy a hydrophobic cleft between two molecules of the human retinoic acid receptor ligand-binding domain. The detergent molecule (Fig. 1a) is clearly visualized in the crystal structure (Fig. 1b) with the cavity apparently being specific for the α -isomer, and the maltose head group forming hydrogen bonds to protein side-chain residues. The detergent acts as a spline, helping to keep the two molecules in a fixed orientation and increasing the contact area (by 38%) to strengthen the interaction. A likely reason for the ability to crystallize macromolecules is their tendency to self-associate in defined structures. Additives or procedures that can initiate the formation of defined structures in solution may be key factors in obtaining macromolecular crystals. Macromolecular crystallographers are on a constant search for the Holy Grail of crystal growth. The use of screening kits and detergents is one approach. Manipulation of the physical environment as an alternative is seen as a more global approach, one that does not have to be tailored to a specific molecule. In recent years the use of microgravity and gels have been investigated. Neither is without problems, but steady progress is being made. Now another method is emerging, the use of high magnetic fields to suppress convective flow. Sato *et al.* [*Acta Cryst. D* **56** (2000), 1079-1083] report measurable improvement in mosaicity and diffraction resolution in crystals of lysozyme grown in a 10 T magnetic field. The *c* axis of the crystals was found to be aligned with the magnetic field (Fig. 2) and the diffraction resolution was increased from 1.3 Å at 0 T to 1.13 Å at 10 T.

This short review highlights a variety of crystallization developments and case studies. Many more are described in greater detail in each issue of *Acta Cryst. D*. The vigorous crystal growth field is poised to achieve the high throughput required in today's structural genomics world.

Marc Pusey, NASA, Huntsville, AL, USA

Naomi Chayen, Imperial College School of Medicine, London, UK

IUCR JOURNALS NEWS

International Conference on Small-Angle Scattering proceedings published

The XIth International Conference on Small-Angle Scattering (SAS99) explored the role of small-angle scattering in a broad range of scientific disciplines concerned with the correlation of structure, interaction, and properties of complex materials. Contributions to the scientific program demonstrated that scattering when complemented with other techniques or when analyzed with physically meaningful computational models provides new insights into structure and dynamics of solids, soft matter, and solutions.



Gernot Kostorz.

Four parallel sessions were required to accommodate the programs in alloys and ceramics, biology, colloids, complex fluids, polymers, polymer processing, surface and interface, theory and technique, and ultra small-angle scattering. The wellattended sessions were a compliment to the insightful work of the Scientific Program Committee in shaping a representative and diverse program from the submitted abstracts. Strong multidisciplinary research programs at universities as well as new opportunities created by the increasing number and diversity of experimental facilities at synchrotrons and next-generation neutron sources attract investigators in all disciplines. The members of the International Advisory Board encouraged the organizers to explore frontiers in low-resolution structure determination and to invite the participation of young investigators. Their innovative research, broad spectrum of interest and enthusiastic participation in discussions is a key factor that gives this unique technique-oriented conference series vitality. After thorough review, 107 papers were accepted for publication. The proceedings of the meeting have been published in Volume **33**, Part 3 Number 1 of the *Journal of Applied Crystallography*. The proceedings were edited by Conference Co-chairs Dieter K. Schneider and Sow-Hsin Chen and Guest Editors Malcolm S. Capel, Benjamin Hsiao, Gernot Kostorz, Jan Skov Pedersen, Peter Timmins and George D. Wignall.

Copies are available at US\$70; for an order form, send your details to as@iucr.org.

IUCr ACTIVITIES

IUCr Commission on International Tables

The main activity of the Commission on *International Tables* is planning, editing, and maintaining the volumes of *International Tables for Crystallography*. The present and future volumes will be typeset from files prepared in standard generalized markup language (sgml).

Details concerning the International Tables and the activities of the commission are available on the home page of the Commission, accessible at the URL: <http://crystal.tau.ac.il/xtal/comit/comit.html> and the description of the commission activities at the Glasgow meeting is accessible at: <http://crystal.tau.ac.il/xtal/comit/ocit99.html>.

Published volumes and new editions

- *Volume A: Space-Group Symmetry*, Editor: Th. Hahn Brief Teaching Edition of Volume A, Editor: Th. Hahn
- *Volume B: Reciprocal Space*, Editor: U. Shmueli
- *Volume C: Mathematical, Physical and Chemical Tables*, Editor: E. Prince and A.J.C. Wilson

Volumes in preparation

- *Volume D: Physical Properties of Crystals*, Editor: A. Authier
- *Volume E: Subperiodic Groups*, Editors: V. Kopsky and D.B. Litvin
- *Volume F: Macromolecular Crystallography*, Editor: M.G. Rossmann and E. Arnold
- *Volume G: Crystallographic Information*, Editor: S. R. Hall and B. McMahon
- *Volume A1: Maximal Subgroups of Space and Plane Groups*, Editor: H. Wondratschek

U. Shmueli

IUCR ACTIVITIES

Crystallographic Nexus Software CD-ROMs

Academics and students in crystallography working in laboratories in the developing world which are isolated from the Internet are invited to register for Crystallographic Nexus Software CD-ROM [1] free of charge.

The ability to produce these CD-ROMs is primarily due to the permission of software and web site custodians; with sponsorship and guidance from the International Council for Science (ICSU) (2), International Union of Crystallography (3) and CCP14 Project for Single Crystal and Powder Diffraction (4).

The Crystallographic Nexus CD-ROM is a virtual Internet on CD-ROM containing Web and FTP sites housing a variety of crystallographic software packages including single crystal software; powder diffraction programs; educational resources and miscellaneous crystallographic information.

Initial CDs will be optimised for MS-DOS and MS-Windows operating systems; but will contain Mac and Linux binaries that can be copied from the CD on these operating systems. The NeXus project is organized by the IUCr Committee on Electronic Publishing, Dissemination and Storage of Information (CEP) which will be responsible for selecting recipients from the requests received. A list of Developing Countries as defined by the OECD is available on the World Wide Web (5).

Requests should be addressed to: Lachlan M.D. Cranswick (CCP14 Secretary), Collaborative Computational Project No 14 (CCP14) for Single Crystal and Powder Diffraction, Synchrotron Light Source, CLRC Daresbury Laboratory, Warrington, WA4 4AD UK, Tel: 44 1925 603703, Fax: 44 1925 603124, E-mail: L.Cranswick@dl.ac.uk, www.ccp14.ac.uk

1. Xtal Nexus CD-ROM homepage at the U. of Geneva: <http://crystalsun1.unige.ch/stxnews/nexus/index.htm>.
2. ICSU (International Council for Science): www.icsu.org
3. IUCr (International Union of Crystallography): www.iucr.org
4. EPSRC funded CCP14 Project (Collaborative Computational Project No 14 for Single Crystal and Powder Diffraction): www.ccp14.ac.uk
5. OECD List of Developing Countries in Alphabetical Order: www.oecd.org/dac/htm/ldc-alfa.htm

IUCR ACTIVITIES

Mike Dacombe: 25 years of service



Mike Dacombe, the Executive Secretary of the IUCr since 1993, has completed 25 years of service with the Union. Mike joined the IUCr as an Editorial Assistant in 1975, having been recruited by the late Jim King, then Executive Secretary, at the time of the World Congress and General Assembly in Amsterdam.

Mike's undergraduate training was in Chemistry and Earth Sciences at the U. of Leeds, from where he joined the Information Dept of BNFL's Metals and Technology Centre. He arrived at the IUCr when *Acta Crystallographica* consisted of just sections *A* and *B*, and the *Journal of Applied Crystallography* was only seven years old. The technical editing staff comprised three people, including Mike. Over the years, the activities of the journals, as well as *International Tables*, steadily expanded and *Acta Crystallographica Section C* was integrated in 1983. During this time, Mike worked on *Acta Crystallographica Sections A* and *B*, eventually taking over responsibility for *C*. In 1986 he was appointed overall Technical Editor. Whilst Technical Editor, Mike oversaw the Union's first steps into the world of computerised typesetting, indexing and manuscript tracking.

In 1993 Mike was appointed Executive Secretary, succeeding Jim King, who died suddenly at the age of 55. The 1990's were eventful under Mike's charge with notable events being the launch of *Acta Crystallographica Section D* in 1993, the launch of *Journal of Synchrotron Radiation* in 1994 and, of course, the 50th Anniversary of the IUCr in 1998. Many crystallographers around the globe will know the name of Mike Dacombe but the members of the Executive Committee, the Journals Commission, and all the Commissions and Committees of the Union know Mike personally as the steady hand and contact for all the IUCr organisational work. Moreover, Mike's diplomatic touch in solving problems is notable.

We congratulate Mike on his achievement of 25 years service with the IUCr; we also send our best wishes for the continued smooth running of the Union's business with not too many problems for the future!

John R. Helliwell

REGIONAL NEWS

The 50th anniversary of the Crystallographic Society of Japan



N. Kato, Reminiscences of P. P. Ewald.

A symposium to celebrate the 50th anniversary of the Crystallographic Society of Japan was held on July 1 in Tokyo. After opening remarks by Fujiko Iwasaki (President of the CrSJ), Yasuhiko Fujii (Chair of the National Committee for Crystallography, The Science Council of Japan), Yuji Ohashi (President of AsCA) and Michiyoshi Tanaka (Vice-president of the IUCr) reviewed the fifty year history and activities of the CrSJ. Emphases was placed on the exceptional quality of Japanese crystallography school founded by Torahiko Terada (1878-1935) and his pupil Shoji Nishikawa (1884-1952), who later became the first president of the CrSJ. Terada had independently discovered the relationship equivalent to the Bragg rule in 1913⁽¹⁾. Nishikawa determined the structure of spinel by using space group theory in 1915⁽²⁾ and was a supervisor of R.W.G. Wyckoff⁽³⁾.



Y. Ohashi, Y. Fujii, N. Kato, F. Iwasaki and M. Tanaka at the 50th anniversary symposium of CrSJ.

K. Osumi, S. Komiya, H. Fukuyama, F. Iwasaki, S. Yokoyama, T. Matsuzaki, T. Nishinaga and S. Kikuta discussed the future of crystallography in the next century and its role in the advancement of space science, physics, chemistry, material science, biology, biochemistry, and pharmacy. Norio Kato (president of IUCr in 1978) delivered the closing remarks, including anecdotes concerning P.P. Ewald.

- 1) Torahiko Terada, 'X-Rays and Crystals', Nature, XCI (1913) 135-136. 'X-Rays and Crystals', Nature, XCI (1913) 213.
- 2) Shoji Nishikawa, 'Structure of some crystals of spinel group', Proc. Tokyo Math.-Phys. Soc. Vol.8 (1915) 199-209.
- 3) Acta Crystallogr. A51(1995)649-650.

Masaki Takata

REGIONAL NEWS

Crystallography in... The Netherlands

J. Kroon (president), A.W.M. Braam, B. Dijkstra, S. Harkema, H. Reynaers, F. Tuinstra, R. Olthof-Hazekamp (secretary), L. Woning are members of the National Committee for Crystallography of The Netherlands. The first five people in this list are also members of the council of the Chemistry Foundation of the Netherlands Research, Dept. Crystal and Structural Chemistry, (NWO-K&S). All universities and industries, having a crystallographic department, are represented in NWO-K&S. Tuinstra, Olthof-Hazekamp, and Woning are the council of the Dutch Crystallographic Association (NVK), an adhering body of the IUCr. The NVK has about 270 members, including PhD students, retired crystallographers and 20 Belgian crystallographers. All interested members are listed in the World Directory of Crystallographers.

Every spring there is a 2-days national meeting organized by the NWO-K&S and in November a 1-day symposium is organised by the NVK. In the year 2000 the NVK meeting will be held in Leuven, Belgium. Every two years there are meetings of the groups on powder diffraction and protein crystallography.

Roeli Olthof-Hazekamp

REGIONAL NEWS

Crystallography in... Russia



L. Atovmyan, V. Belsky, W. L. Duax, and L. A. Aslanov at the Chernogolovka meeting on Crystal Chemistry.

The Russian Foundation of Basic Research (RFBR) supports crystallographic research in chemistry, physics, earth sciences, and biology. There are currently 27 grants supporting organic and inorganic crystal-chemistry and about 40 on the crystallography of minerals. This does not cover all researchers of crystallographic significance. In its Chemistry section alone, 258 of a total of 1149 grants include varying levels of crystallographic investigation.

RFBR supports international joint research groups together with INTAS (European Union), DFG(Germany), CNRS (France), and NSFC (People Republic China). Crystallography is represented in these grants as well.

RFBR supports the organization of scientific conferences such as the Second National Crystal-Chemical Conference in Chernogolovka in May, 2000. Airfare for Russian scientists who are invited to speak at international conferences is provided with some preferences given to young scientists.

Oleg A. Dyachenko, L.A. Aslanov

MEETING REPORT

Crystal chemistry in Russia



Attendees at the 2nd Russian Conference on Crystal Chemistry wave farewell before boarding a space shuttle for an out of this world excursion. That's Virtual Reality for you.

The second Russian National Conference on Crystal Chemistry, held May 22-26, 2000 in Chernogolovka, near Moscow, was organized by the Section of Crystal Chemistry of the Scientific Council on Structure and Reactivity and the Inst. of Problems of Chemical Physics of Russian Academy of Sciences with sponsorship from the Russian Foundation of Basic Research, ICDD, and Bruker. There were about 300 oral and poster presentations divided into seven sections - organic, inorganic and coordination crystal chemistry, structure-properties correlation, chemical bonding, solid state reactions, and dynamic crystal chemistry. The participants were from all parts of Russian and former Soviet Union republics. There were lecturers from USA, Japan, France, Germany, Israel, and Mexico. The opening lecture was delivered by the patriarch of Russian crystal chemistry, Goergy Bokii. V. Belsky was Chairman of the Program committee and L. Atovuyan was Chairman of the Local Committee.



MEETING REPORT

Seminar on Crystallography in India

The XXX National Seminar on Crystallography was held June 28-30, 2000 in Tirupati, India. R. Chidambaram, Chairman of the Atomic Energy Commission and Secretary to Govt. of India, Dept. of Atomic Energy, Inaugurated the seminar and delivered the Keynote address. O.N. Srivastava, Chairman of the Nat'l Committee for Crystallography (INSA) addressed the gathering. Many eminent scientists, such as M. Viswamitra, Dr. Krishanlal, M. Ramanatham, V. Pattabhi, T.S. Cameron, T.N. Guru Rao, and M.R.N. Mruthy attended the meeting.

There were 276 abstracts received, 33 invited talks were delivered and 225 delegates participated in Oral and Poster presentations. Dr. Chidambaram concluded the seminar announcing BARC, Mumbai as the next venue for the seminar.



M. Krishnaiah

MEETING REPORT

Software Fayre

Throughout the IUCr Glasgow Congress, a Software Fayre was held to allow software authors and users to interact with the various freely available packages useful to Crystallographers. Thanks to the generosity of SGI and Compaq and the help of the organising committee, attendees had access to 3 Silicon Graphics O2s, 2 Compaq PCs running Redhat Linux and 5 Compaq PCs running Window95; as well as an overhead computer projector for demonstrating software to larger crowds.

Small-molecule single-crystal software

J. Gallagher demonstrated the ORTEX for Windows single crystal suite (based around Shelx for solution and refinement); S. Hall and B. Skelton, the XTAL single crystal solution and refinement suite running on UNIX and Windows; P. Mallinson and T. Richter, the 'Project XD' Charge Density Software; D. Watkin and R. Cooper the new GUI based CRYSTALS refinement suite for Windows; L. Farrugia the WinGX for Windows suite (based around Shelxs, Sir and Dirdif for solution and Shelxl for refinement). R. Spagna demonstrated the combination of using Sir and CAOS (Crystal Analysis Operating System) to solve (Sir for direct methods, CAOS for Patterson methods) and CAOS for refining structures; M. Dusek, the JANA98 program (UNIX and PC) for refinement of ordinary and modulated structures; P. and G. Beurskens the Patterson methods and difference direct methods based DIRDIF structure solution package (UNIX and PC). R. de Gelder showed how easy it is to compile and install the the direct methods CRUNCH structure solution package under UNIX and Linux for handling difficult structures. F. Pavelcik demonstrated the Patterson methods based XFPA structure solution program (UNIX and PC) and T. Spek the Platon/'System S' single crystal suite (UNIX/Linux) (Shelxs, Sir, Dirdif and Crunch for structure solution, Shelxl for refinement and powerful Platon tools).

Powder diffraction

Demonstrations included: R. Shirley on the CRYSFIRE powder indexing suite who successfully indexed some Protein powder diffraction data provided by Bob von Dreele; A. Le Bail on solving structures from powder diffraction data using the Monte Carlo based methods incorporated into the ESPOIR software; and J. Rodriguez-Carvajal showed the latest foolproof Rietveld friendly plug-in, the 'GFOURIER' Fourier Map generation and display software.

Protein/macromolecular crystallography

On the protein side, software demonstrations included P. Williams on the XtalView program for UNIX (fitting electron density maps and solving structures by MIR and MAD software); I. Uzon applying Shelxpro/Shelxl for refinement of protein structures (with the possibility of using XtalView to view the maps); M. Szebenyi, the MacCHESS Software/ GUI for processing protein crystallographic data using DPS programs, mosflm, and some CCP4 programs; and a demonstration of MICE (Molecular Sciences and Interaction Environments). B. von Dreele also showed GSAS in action which is now also used powder diffraction refinement of Protein structures, with maps and structure linking into the Swiss-PDB Viewer.

Databases, structure manipulation, diffuse scattering and educational software

A. Hewat used one of the SGI O2s to demonstrate the web-based ICSD (Inorganic Crystal Structure Database) and a Linux machine was applied for a DISCUS diffuse scattering/ crystallographic teaching demonstration by T. Proffen and R. Neder. PowderCell for Windows and Cryscon for Windows were shown as effective tools for dealing with structure transformations, including classical phase transformations. Most of the above mentioned software is available for download via the internet for anyone to try out.

The powder diffraction and single crystal software is also mirrored (where possible) on the CCP14 website and its mirrors (<http://www.ccp14.ac.uk>). Thus there is no excuse not to try some of these tools and check their suitability to assist in high quality crystallographic analysis.

Lachlan Cranswick

Web addresses where expanded descriptions of all programs described and demonstrated can be found on the BCA website (<http://gordon.cryst.bbk.ac.uk/BCA/index.html>) from which this article was taken.

MEETING REPORT

ECM2000



Speakers in the microsymposia on Telepresence Internet and Remote Experiment Control at the ECM 2000 meeting in Nancy include (front row) L.M.O. Cranswick, R. Spagna, M. Ianigro, and (back row) A.W. Hewat, T. Proffen and L. Lutterotti.

BOOK REVIEW

Dorothy Hodgkin - a life

Dorothy! You recognize the face. You know the name. But have you read the book?



This book, the 400-page biography of Dorothy Hodgkin, is a superb portrait, in fascinating detail, of the life-history, experiences and personality of this unique individual. The book is so well written, so readable and, in its style, so delightfully in harmony with the life being described, that it is a real treat to read, a fitting tribute to an outstanding and memorable person.

While the context of this book is the development of crystallography, during the initial three decades of its application to organic structures, the focus of the book is simply Dorothy herself – the person – how she started life, how she worked her way into a scientific career, battled against the odds that were stacked against women in those days, quietly established herself amongst the top echelon of structural crystallographers and eventually developed an international reputation and influence. Her crystallography was outstanding (it was Dorothy's first and most passionate love) but her personality is what many of us remember most.

Crystallographers have a special bond with Dorothy. She was one of us, absolutely, in the thick of our activities from the beginning of our crystallographic science and community (the 1940's) until her death at the age of 84. She was a familiar face in our conferences. Encountering her there - an unobtrusive, gentle, slow moving, courteous lady, no one would suspect that she was particularly important. She was the mother of three children and she was also the person who, with Bernal, obtained the first-ever X-ray diffraction picture from crystalline protein (pepsin, in 1934). She was the leader of the group that elucidated the structure of the first antibiotic, penicillin (in the early 1940s) and was honoured with membership of the Royal Society of London, at the youthful age of 37 (1947). A decade later, she had capped the penicillin success with the structure of Vitamin B12 (1957); and another decade later, the B12 triumph was capped with that of the structure of insulin. She was awarded the Nobel Prize in Chemistry 1964. Her list of students, colleagues and co-workers includes the names of over 110 men and women from over 20 countries. The British Government awarded her the Order of Merit (OM) in 1965, the highest, and rarest British civilian honour. The British Post Office issued a stamp with her portrait: one of four 'women of achievement' in 1996. She had Honorary Membership in eight National Academies, and had received honorary Degrees from 21 Universities. She was the President of the IUCr from 1972-75. Such were the accomplishments of this gentle and lovable lady, 'our Dorothy'.

How did all this happen?

Was it sheer genius? Or the consequence of historical accidents - being in the right place at the right time and knowing the right people? In fact, it was both of these; and this biography by Georgina Ferry expertly takes us through Dorothy's development, from the innocence and excitement of childhood, to the serious and painful traumas of political involvement.

It is now six years since Dorothy died. There have been dozens of obituaries and review articles in the scientific journals and lay press. Even if you have seen these articles, I recommend that you read this rich, full and entertaining biography. What is special about Ferry's book is the style of the narrative and the inclusion of so many delightful details and memorable quotations from Dorothy's letters and notes. Ferry brings Dorothy to life again with her naturalness, informality, and emotional strength intact. Each chapter is headed with a typical Dorothy quote. (Chap. 1) 'It is a rather rackety childhood in a way' and (Chap. 4) 'It'll serve me absolutely right if the thing is all wrong'. Lest the quotes be misunderstood, each chapter has a normal subheading, such as (Chap. 4) 'Oxford, insulin and Thomas'. These chapter headings are just one way in which Georgina's story re-creates Dorothy's character in the biography.

Sheer genius, or good fortune?

There was continuous interplay between Dorothy's genius and the opportunities she enjoyed because of her background and circumstances. Her gift for intellectual adventure was actively encouraged by her mother – rare for a young girl in those days. Dorothy's mother nurtured her daughter's intellectual growth and was prepared to allow her almost unlimited freedom. Another instance of serendipity occurred when one of her father's friends in Cairo, a chemist, Dr. Joseph, was so impressed by her interest in minerals that he gave her a set of chemicals with which to analyze them. She was particularly enchanted by crystals. With this stimulus and encouragement, she threw herself into the pursuit of the science behind her crystals. Her mother bought her W.H. Bragg's book, 'Concerning the Nature of Things'; and 'The Fundamentals of Biochemistry' by T.R. Parsons and she extracted the necessary organic chemistry from the Encyclopedia Britannica. Her childhood love of crystals never left her.

That Dorothy's parents were so academically supportive was a fundamental factor in her career choice. Her father had graduated from Oxford, and at the age of 17 she was determined to get into Oxford University. Alas, her acceptance at Somerville College, Oxford was delayed a year while she mastered Latin and other requirements. After graduation from Oxford, she benefited again from the help, advice and assistance of well-placed people, including her old friend, Dr. Joseph. As a result she went to Cambridge in 1932, to work with Bernal. Association with Bernal fundamentally influenced the whole of her subsequent career, steering her interests toward the application of X-ray crystallography to biological structures. Ferry's numerous quotations from personal letters of that time give a vivid picture of the whirl of emotions prior to this move.

Dorothy was with Bernal in Cambridge for only two years (1932-1934) when she was invited by Somerville College to return to Oxford as their Chemistry Instructor where she soon became Lecturer, and then a Fellow. But the friendship with Bernal, and his influence remained.

Friendships in Oxford had crucial significance. In 1934, Robert Robinson gave her crystals of insulin, from which she quickly got very beautiful, but very complex X-ray diffraction pictures. Seven years later, her friend, Ernst Chain, met in the street, told her excitedly how important it would be to determine the structure of penicillin, which was the subject of great controversy and confusion. Soon she was fully engaged in determining its crystal structure. As a result of the penicillin work she made FRS (1947). Her friend Lester Smith brought her some beautiful, cherry-red crystals of Vitamin B₁₂, the structure of which she mapped in 1957, and that accomplishment led to the award of the Nobel Prize. The crystals of insulin became the bases of her most sensational achievement (in 1969). To each successive opportunity, Dorothy applied the full force of her insight, skill, chemical knowledge, and feminine intuition; together with her almost unlimited patience, and these qualities gave her one success after another. Friendships were central to Dorothy's life. They became increasingly international as she began in the 1980s to exert her influence for peace in international relations.

There will never be another Dorothy Hodgkin. Such unique conjunctions of genius and circumstance do not repeat. We can be grateful to have known her, as we have done. We can be grateful too for this fine biography of such an exceptional, successful and loveable person.

John H. Robertson

Ferry's biography, which has been available in Europe for two years is now going to be available in the North American continent from Cold Spring Harbour Laboratory Press. For Europe, and all other countries, Granta still have good stocks of both the hard cover edition (at £20) and the softback (at £10) £ both very good value for their price.



Clockwise from upper left Dorothy with Linus Pauling in Anlonia in 1977; surrounded by women crystallographers (including Carol Huber and Anita Lewit-Bentley) at the ACA meeting in Philadelphia in 1989; at an IUCr International Congress meeting in Beijing with Jack Dunitz and Bill Lipscomb in 1986; with a younger Jack Dunitz visiting Niagara Falls in Ontario, Canada, 1981; and in the center as she looked at graduation from Oxford in 1932.

FEATURE ARTICLE

Women in science and crystallography



Women, gathered to honor Gabrielle Donnay at a symposium organized by Suzanne Fortier at the ACA meeting in Hamilton Ontario in 1986, including past ACA president Jenny Glusker and future ACA presidents Helen Berman, Connie Chidester, Penny Coddington, and Judy Flippen-Anderson.

Unfortunately, a disproportionate amount of the material that appears here (and elsewhere in the Newsletter) is drawn from English language publications. This is more a consequence of the Editors' language limitation rather than his national bias. Readers everywhere are invited to submit news items, letters, and observations on crystallography in their country for possible inclusion in the Newsletter. -

W.L. Duax

In 1998, women earned their largest percentage of research doctoral degrees in US history, according to a survey performed for NSF. Women received 41.8 percent of all doctorates granted in the United States in 1998. While increases occurred in the number of degrees granted women in the physical sciences and engineering, the percentages remained small: 23.7 and 13 percent of these degrees, respectively, went to women.

In May, 2000, C&EN published the results of a survey of women in the top levels of management in the chemical industry. The results indicated dismal representation of women in upper management. Of 1,641 tenure-track positions at the top 50 universities in the US, 172 - about 10% - are held by women and just 6% of full professors. Thirteen institutions have no women full professors, 19 have no women associate professors, and 15 have no women assistant professors.

Madeleine Jacobs, Editor-in-chief, C&EN, Sept. 25, 2000

Michael Smith (U. of British Columbia), 1993 Nobel Laureate in Chemistry, donated \$175,000 of his approximately \$525,000 award to Canadian Women in Science & Technology, a group that encourages women to take up careers in science.

In what she titled as 'a very personal account' of Chemical Crystallography in Neuchâtel, Switzerland 1971-1995, Helen Stoeckli-Evans noted that in 1995 she was the only female professor of chemistry in Switzerland and that although she had the title of Professor Associate, she was not a member of the faculty. She commented that 'within the Chemistry Institute I have always been treated fairly. For a woman in science to obtain a faculty position she must be extremely ambitious and motivated and of course twice as good as her male colleagues. To combine all this with a family, children and a home to run is nothing short of a miracle and those that achieve it should be supported and encouraged. I am in an extremely privileged position here in Neuchâtel and appreciate it greatly.'

Stoeckli-Evans attributed her success, at least in part, to her husband's position at Neuchâtel (despite the attendant mutterings of nepotism) [Marie Curie had similar circumstances. Pierre Curie had a modest position and a laboratory where Marie was permitted to work; it is unlikely that she would otherwise have found a place to do independent research. *ed*]

In the late 1940s when the Westinghouse Science Talent Search ceremonies were held at the Cosmos Club in Washington, D.C., girls were not permitted to enter the building by the front door.

From a review of Women Scientists in America: Before Affirmative Action, 1940-1972, Margaret W. Rossiter by Caroline L. Herzenberg, C&EN, May 6, 1996

When the career paths of men and women who held prestigious post-doctoral fellowships between the mid-1950's and the mid-1980s were followed, it was found that with the exception of biological scientists, male scientists in positions of power (doctoral and postdoctoral advisers and tenured professors) often harmed women's scientific careers, both intentionally and unintentionally. Some overt forms of discrimination have lessened in the past 30 years, but others have merely been hidden in the face of federal requirements. Subtle barriers persist, such as excluding women from the informal venues where inside information is exchanged. The authors note that despite increases in skill and knowledge, women continue to lack the advantages that come from being included in powerful networks. How male superiors choose to exercise their power makes a difference in how a woman experiences science and in how her career evolves.

From a review of Gender Differences in Science Careers: The Project Access Study, Gerhard Sonnert with Gerald Holton by Henry Etzkowitz, C&EN, August 28, 1995

There's too much evidence to suggest that, if left to its own devices, the status quo won't change - individuals' goodwill has never been enough. Maria Goeppert Mayer never had a position commensurate with her status until after she won a Nobel Prize. How could this happen if merit were so readily recognized by the system?

Irene Newhouse, Kihei, Hawaii, C&EN June 12, 2000

Drawing more women and minorities into science is no longer so much about righting the wrongs of the past as it is about developing talent for the next century. Recent estimates indicate that between the mid 1980s and the year 2000, the majority of growth in the labor force will come from the entry of women, people of color, and immigrants. In an international, stridently competitive 'information age', we have to mobilize all of the latent talent in this new work force.

M.R.C. Greenwood, Science, Vol 271, March 29, 1996

NOTICE

First woman CrSJ President elected



Fujiko Iwasaki (U. of Electro-Communications) was elected president of the CrSJ in April 2000. She is the first woman president of the CrSJ. Other new members of the Executive Committee include: General Secretary: **Akio Takenaka**; Treasurer: **Shigeru Ohba**; Chair of the Committee on Meeting and School of Crystallography: **Yasushi Kai**; Chair of the Committee on Int'l Communication: **Masaki Takata**; Chair of the Committee on Data Base and Information: **Yoshinori Satow**; Chair of the Committee on Journal of the CrSJ: **Satoshi Sasaki**.

AWARDS AND PRIZES

2000 Hans Neurath Award



Janet M. Thornton received the 2000 Hans Neurath Award of the Protein Society. Among Dr. Thornton's most notable achievements are developing a powerful classification system for protein structures, new methods for protein fold recognition by threading; and novel technology to assess the accuracy of protein structures. She received her PhD from King's College of the U. of London (1973), was appointed Professor of Biomolecular Structure at University College of London (1990), and has held the Bernal Chair at this institution since 1998. She is director of the BBSRC Centre for Structural Biology at Birkbeck. She became a fellow of the Royal Society in 1999.

AWARDS AND PRIZES

Croatian State awards



Boris Kamenar (University of Zagreb, Croatia), the Chair of the Croatian Crystallographic Association, received the highest State Award for all his outstanding achievements in Organometallic Structural Chemistry and for promotion of Crystallography during his scientific career. **Branko Kaitner**, University of Zagreb, Croatia, received the Annual State Award for 1999 for his recent scientific achievements in Structural Chemistry.

AWARDS AND PRIZES

US Biophysical Society 2001 awards

Frederic M. Richards received the Distinguished Service Award for service in the field of biophysics.

Jane Richardson received The Emily Gray Award for significant contributions to education in biophysics.

The award winners will present lectures at the 2001 Annual Meeting in Boston, MA.

AWARDS AND PRIZES

US National Academy of Sciences awards

Wayne A. Hendrickson (Columbia U.) received the Alexander Hollaender Award in Biophysics. **Isabella L. Karle** (Naval Research Lab) received the NAS Award in Chemical Sciences.

NOTICE

UK Royal Society 2000 Fellows

Cyrus Chothia and **Ian A. Wilson** have been made Fellows of the Royal Society of the UK. **Cyrus Chothia** (Medical Research Council Laboratory of Molecular Biology, Cambridge, England), has shown how the amino acid sequences of proteins determine their structure, function, and evolution. From an analysis of their structural regularities, he developed a classification of protein structures that is now in general use. His picture of protein evolution suggests how protein diverge and gain new functions. He has contributed to the understanding of how their apparently limited set of slightly different structures allows immunoglobulin to recognize an almost limitless variety of different antigens. **Ian A. Wilson** (Skaggs Inst. for Chemical Biology, Scripps Research Inst., La Jolla, CA) is noted for structural studies that have led to significant advances in understanding molecular recognition in the immune system and signaling by cytokine hormone receptors. His achievements include the structures of the T-cell receptor and its complex with a major histocompatibility complex peptide, the erythropoietin receptor, antibody-antigen complexes, catalytic antibody mechanisms, and the influenza virus hemagglutinin. His work has attracted recognition for the elegance of the structural solution to important biological problems.

from the BCA Newsletter

AWARDS AND PRIZES

Congratulations to ...

Ivan Bernal received an Alexander von Humboldt US Senior Scientist Award at the Technical U. of Munich as Visiting Professor. He participated in the design of a neutron diffraction instrument to be located in their new reactor (Forschungs-Reaktor München II (FRM-II)) to be completed in the Fall of 2001. This reactor will have ten ports and approximately the same beam intensity at the sample as the Brookhaven reactor when it was operating at its peak. Its source will be a massive, single uranium rod, and the diffractometer will have as its detector a curved plate. The instrument will be manufactured by Enraf-Nonius.

Yale biochemist **Jennifer Doudna** is this year's winner of the Alan T. Waterman Prize: \$500,000 from the National Science Foundation to a promising young researcher. Doudna, 36, a Howard Hughes professor of molecular biophysics and biochemistry, is the third female winner in the Waterman's 25-year history. She uses X-ray crystallography and biochemical techniques to show how RNA can act like an enzyme to catalyze specific biochemical reactions.

Douglas C. Rees, Howard Hughes Medical Inst. and California Inst. of Technology, a previous winner of the Sidhu Award from the Pittsburg Diffraction Society, was elected to the National Academy of Sciences in recognition of his distinguished and continuing achievements in original research.

NOTICE

European Crystallographic Association elections



Claude Lecomte.

The new ECA Executive Committee was elected at the Council meeting in Nancy: President: **Claude Lecomte**, Vice-President: **Paul T. Beurskens**, Secretary: **Giuseppe Filippini**, Treasurer: **Maria T. Duarte**, Members: **Eleanor J. Dodson**, **Mariusz Jaskolski**, and **Davide Viterbo**. The Election of new ECA Councillors to represent Individual Members in the ECA Council were based on votes representing about 45% of the Individual Members. Because the number of the Individual Members exceeds 400, four Councilors have been elected. They are: **Carlo Mealli**, **Keith Wilson**, **Paola Spadon** and **Paola Gilli**.

MISCELLANY

You can fold some of the proteins all of the time

A technique for identifying folding patterns of proteins using mass spectrometry that is potentially faster and requires less sample than X-ray crystallographic or NMR methods has been developed by B.W. Gibson and I.D. Kuntz. They believe the time needed to determine the fold family of a protein can be reduced to one week and that less than 10mg of protein may be required to elucidate macromolecular interactions, and multiple conformational states, and to contribute to the design of protein mimetics.

C&EN, June 5, 2000

MISCELLANY

Good science

Five diagnostic features of good science are: repeatability; economy (simple and aesthetically pleasing); mensuration (proper measurement); heuristics (stimulates further discovery); and consilience (connected and proved consistent with other good science). The work of real science is hard and often for long intervals frustrating. If you choose an academic career you will need 40 hours a week to perform teaching and administrative duties, another 20 hours to conduct respectable research and still another 20 hours to accomplish really important research. Advice to the novice scientist: There is no fixed way to make and establish a scientific discovery. Throw everything you can at the subject, so long as the procedures can be duplicated by others. Consider repeated observations of a physical event under varying circumstances, experiments in different modes and styles, correlation of supposed causes and effects, statistical analyses to reject null hypotheses (those deliberately raised to threaten the conclusion), logical arguments, attention to detail and consistency with results published by others.

Edward O. Wilson

American Scientist 86, Jan./Feb. 1998

MISCELLANY

Gone in 60 seconds



Members of the IUCr Executive Committee in Action. The first three readers to identify all five correctly will receive a copy of the Transactions of the American Crystallographic Association, Volume 33, *Crystal Engineering*, or Volume 34, *Two Decades of Synchrotron Radiation Research*.

NOTICE

18th ECM Conference publications



Materials Structure in Chemistry, Biology, Physics and Technology, vol. **6**, no. 2 1999, 87 pages, ISSN 1211-5894. 22 reviewed papers on special topics presented on ECM-18.

Advances in Structure Analysis, Editors R. Kuzel, J. Jasek, 510 pages, issued November 2000. Selected full papers on general topics presented at ECM-18: materials structure and physics (9 papers), chemical crystallography (9 papers), methods of structure determination (6 papers), biology (3 papers), symmetry (2 papers). All contributions have been reviewed. Authors: J. W. White, P. Klimanek, H. J. Bunge, P. Barnes, C. Landron, Gu Nanju, R.I. Barabash, S. V. Starenchenko, I.V. Alexandrov, M. Steinhart, V. Kaucic, A. Le Bail, K. D. M. Harris, F. H. Herbstein, S. V. Krivovichev, G. A. Geguzina, P. Capková, K. Yoshimura, K. S. Byram, D. Weigel, V. Kopsky, M.G. Munteanu, A. Deriu, K. Vlahovicek, C.M. Weeks, A. Podjarny, C. Gilmore, V. Lamzin, C. Giacovazzo, V. Y. Lunin and other authors.

CD-search (Search Java applets). Searchable list of participants with full addresses, in many cases with E-mail addresses, phone and fax numbers, WWW pages and a few personal photos. Search in all abstracts for words and their combination with word highlighting (searched words are highlighted in the documents found).

For more information and to order, contact <http://krystal.karlov.mff.cuni.cz/xray/>.

MISCELLANY

19th ECM database

As part of the 19th European Crystallographic Meeting, INIST-CNRS in partnership with the LCM3B (Lab. de Crystallographie et de Modelisation des Materiaux Mineraux et Biologiques) provides on its web site free access to a set of 18 bibliographic and informetric databases derived from the main topics of the meeting.



The walking and drinking team in the Vosges mountains at ECM19.

MISCELLANY

The importance of W. H. Bragg

As a 'scientific grandson' of W.H. Bragg (via J.J. Robertson), I have been disappointed that the senior Bragg's role in the development of X-ray crystallography has tended to be played down. The development of the subject depended on the experience W.H. Bragg gained as Professor of Mathematics and Experimental Physics at Adelaide University in South Australia. Bragg was appointed to the chair in 1885 to build a department. At the age of 42 he began research on α -particles. He acquired experience in the procedures for determining the intensities of beams of such particles using ionization chambers. He was elected FRS in 1907, and in 1909, he accepted appointment to the chair of physics at Leeds University.¹

During the summer of 1912, father and son had discussions on the recent observations of Friedrich and Knipping and on von Laue's interpretation. When W.L. Bragg, returned to Cambridge, he deduced the relationship, $n\lambda = 2d\sin\theta$. It became evident that the relationship was 3 dimensional and was associated with 3 parameters necessary to adjust a specific plane to the correct orientation for an X-ray reflection to occur. The problem became (a) how to orient a crystal so that a given hkl plane was in the appropriate orientation and (b) how to measure the intensity of the reflected X-ray beam. Step (a) was well known to mineralogical crystallographers familiar with the optical goniometer. Step (b) had, till then, been based on the use of photographic plates. At this juncture, the critical role of W.H. Bragg and his familiarity with ionization chambers is evident.²

With the expertise of Father Bragg, the ionization spectrometer (essentially the later X-ray diffractometer) was created. With the excellent energy and intensity resolution of the new instrument, father and son were able to study scan procedures, the relevance of integrated intensity, etc., the prelude to structure determination of simple crystals.³

Without Father Bragg's skills, the early development of X-ray crystallography could have been much slower, and, indeed, might have occurred elsewhere.

[1] Jenkin, J.G. (1986). *The Bragg Family in Adelaide: A Pictorial Celebration*. The University of Adelaide Foundation in conjunction with La Trobe University.

[2] Caroe, GM. (1978). *William Henry Bragg 1862-1942 Man and Scientist*. Cambridge University Press, pp. 74-75

[3] Bragg, W.H. (1914). *The Intensity of Reflexion of X-rays by Crystals*. *Philos. Mag.* **27**, 881-899. [Reproduced in *Acta Cryst.* (1969), **A25**, 3-11].

A. McL. Mathieson

MISCELLANY

The structured world of Oxford

For me as a post-graduate student, the Oxford Laboratory of Dorothy Hodgkin in the mid 1960s seemed like the center of the world. Dorothy had just been given the Nobel Prize. Distinguished crystallographers from all over the world visited to talk about vitamin B12 and to ask of progress with insulin. Young researchers joined from USA, China, India, Chile, New Zealand, Australia, Canada and all over Europe, eager to participate in the excitement. The successful lysozyme team of David Phillips moved to Oxford in 1966 and those working on insulin relocated alongside in Old Physiology. It was a very stimulating environment for a young scientist. In 1969, thirty five years after Dorothy had observed the first diffraction from rhombohedral insulin crystals, Guy and Eleanor Dodson, Ted Baker, M. Vijayan and I were lucky to be around when the insulin structure was finally solved, the first protein hormone to be successfully subjected to X-ray analysis. The excitement intensified again, with interest from the international scientific community and the press. Nobel Prize winners Perutz, Kendrew, Sanger, Anfinsen and many others came to see Dorothy and we were asked to write reviews and give lectures at prestigious meetings.

T. Blundell, July 98 Nature Structural Biology

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MISCELLANY

The crystallographic tourist in the Antarctic

Durward Cruickshank on Jan. 18, 1998 went on a cruise to the Antarctic Peninsula studying the charts and noticed a region called Crystal Sound, off the west coast of the peninsula.



Durward Cruickshank and Neil Issacs, the past, current and only holders of the Joseph Black Chair in the Dept of Chemistry at the University of Glasgow at the Kelvingrove Art Gallery and Museum in Glasgow. On looking more closely I recognized some rather familiar names given to the little islands and rocks in the Sound: Bragg, Dennison, Bernal, Fowler, Pauling, Owston, Shull, Wollan, Levy, Peterson. Thanks to help from the British Antarctic Survey and the Scott Polar Research Institute, both in Cambridge, and with some assistance from Frank Allen and Kate Crennell, I eventually learnt how these bleak places got their names. The Antarctic Place-names Committee decided to use the names of pioneers in techniques which have helped in the elucidation of Antarctic problems. Glaciologists are obvious choices, and within that group the names of the investigators of the structure of ice crystals were chosen for features in Crystal Sound.

Dr Brian Roberts (1912-1978) in an article 'Glaciologists and Antarctic Placenames', published in *Ice* lists over 100 glaciologists and their achievements e.g.

- Perutz Glacier 67° 37' S, 66° 25' W. M. F. Perutz (GB) b 1914; important studies of mechanism of glacier flow.
- Bragg Islands 66° 28' S, 66° 27' W. Sir W.H. Bragg (GB) 1862-1942; physicist, interpreted X-ray measurements to give location of oxygen atoms in structure of ice.
- Shull Rocks 66° 27' S, 66° 40' W. C. G. Shull (USA) b. 1915; physicist, neutron diffraction to determine position of hydrogen atoms in ice.

R. W. James FRS (1891-1964), colleague of W.L. Bragg and author of *The Optical Principles of the Diffraction of X-Rays*, was a member of the legendary Shackleton expedition of 1914-1916. James' most distinguished student is well known to the BCA: Sir Aaron Klug OM, President of the Royal Society and winner of the Nobel Prize in Chemistry in 1982 for his development of crystallographic electron microscopy and the structures of nucleic acid-protein complexes.

Durward Cruickshank

MISCELLANY

The mechanism of Beevers-Lipson strips

Today, when Fourier transforms on several thousand data items for large, three dimensional unit cells at a resolution of about 0.3 Å require less time than it takes to gulp down a cup of coffee, it is difficult to imagine the size of the task confronting early crystallographers, where this operation was almost unthinkable. After all, even a two dimensional summation of: $S \{A \cos 2\pi (hx+ky) + B \sin 2\pi (hx+ky)\}$ for 500 data items into 2000 points requires 106 summations, let alone any work required to calculate the trigonometric functions! The boxes of strips themselves have virtually disappeared although they were once almost universal in the crystallographic community. A handsome box still survives in the Clarendon Lab at Oxford U. The great contribution of Beevers and Lipson in 1936 was twofold: to simplify the calculations greatly by factorizing the trigonometric expressions to reduce the two dimensional calculations to many fewer one dimensional ones, and to provide a convenient technique for carrying out the summations - the strips themselves.

Some people used mechanical calculators for the sums, but most found it far quicker and more accurate to use mental arithmetic, a skill more widely found then than now.

Bob Gould

From the BCA Newsletter, Dec. 1998

OBITUARY

G. A. Jeffrey - a note

Dr Carrondo's excellent obituary of George, or 'Jeff' as we used to call him ([Newsletter 8-2](#) p.27) does not mention his early career in any detail and I thought that this might be of interest to younger Crystallographers.

I first met Jeff when I started as a research student under E.G. Cox (later Sir Gordon) in 1942. I had migrated from Industry under a Scholarship awarded by the British Rubber Producers Research Association (BRPRA). Jeff was a member of their staff who worked under Cox both on Rubber and on explosives for the Ministry of Supply at Birmingham.

Jeff was working on the structure of Geranylamine Hydrochloride and acted as my mentor in work on Pentaerythritol Tetranitrate. As a physicist and engineer I was particularly interested in improving computational methods which were, at that time, very primitive. Jeff entered with enthusiasm into my improvements and we made an excellent team. In 1944 we both migrated to the BRPRA labs in Welwin Garden City where we shared an office. With the encouragement of Johnny Wilson the Director I was encouraged to develop digital computers whilst Jeff concentrated on chemical matters. A major joint effort was to use IBM punched card equipment to speed up Fourier Analysis and Synthesis in which we used the services provided by L. J Comrie.

We both wished for academic appointments and encouraged each other by, for example, suspending toy Chairs over each others desks. When work proceeded well the Chairs were lowered but a slack period caused a rise to the ceiling. After Jeff and Maureen married and produced their daughter Susan I was able to help them to have fun by minding the baby in the office, I remember constructing a cot rocker from a pair of retort stands and a stirrer motor.

Jeff was appointed to a teaching post in Gordon Cox's department at Leeds University and I moved to a Fellowship at Birkbeck College, London. At Leeds, Jeff was largely responsible for one of the first Crystallographic computing units in England: The Ferranti Pegasus machine. This was nicknamed Lucifer and was housed in a disused Chapel.

Shortly afterwards Jeff moved to Pittsburgh and later I accepted a post in Canada. My last face to face meeting with Jeff was at Susan's wedding. I was shocked to hear of his last illness and death. A dreadful end to a splendid person, a fine scientist and a good friend.

Donald Booth

OBITUARY

Peter Goodman (1928-1999)

Peter Goodman's fundamental contributions in the field of symmetry analysis have found widespread industrial application, in this case extending from metallurgy to microelectronics and from the characterization of minerals to the fabrication of ceramics. Outstanding among his contributions was the use of the convergent incident beam, a technique in electron diffraction to study bonding and determine the presence or absence of a centre of inversion, to analyze the non-symmorphic groups and to determine chirality. Peter had passion for the graphic arts and a deep humour and a wry sympathy for human frailty. He served as chairman of the IUCr Commission on Electron Diffraction, edited *Fifty Years of Electron Diffraction*, organized a variety of conferences and, memorably, wrote the definitive chapter on space group determination by electron diffraction.

Alex Moody, SCA Newsletter, No. 44, Feb 2000