

INTERNATIONAL UNION OF CRYSTALLOGRAPHY

IUCr Newsletter

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Original article text and available illustrations

Contents

Letter from the President

Letter from the President	3
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IUCr journals news

Molecular shapes from small-angle X-ray scattering: extension of the theory to higher scattering angles	5
High-pressure crystal structure of the non-linear optical compound BiB3O6 from two-dimensional powder diffraction data	6
The absolute configuration of 1-epialexine hemihydrate	7
De novo sulfur SAD phasing of the lysosomal 66.3 kDa protein from mouse	8
5-[[[(3R,5aS,6R,8aS,9R,10S,12R,12aR)-3,6,9- Trimethylperhydro-3,12-epoxy-1,2-dioxepino[4,3- i]isochromen-10-yl]-oxymethyl}benzene-1,3-diol	9
The structure of NMB1585, a MarR-family regulator from <i>Neisseria meningitidis</i>	10
Structural changes in nanocrystalline mackinawite (FeS) at high pressure	11
Capturing molecular structural dynamics by 100 ps time-resolved X-ray absorption spectroscopy	12

Special report

Crystallography in Great Britain and Ireland	13
--	----

Awards and prizes

CrSJ 2008 Awards	30
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LETTER FROM THE PRESIDENT

Letter from the President



Sine Larsen

This letter is devoted to an important ingredient of scientific life, namely money. Most science requires financial support from external sources and many scientists spend a significant amount of their time writing grant applications in order to obtain the funding necessary for their research. The grants allow purchase of state-of-the-art equipment and payment of younger researchers, and provide the basis for many of the exciting scientific achievements that are presented at conferences and published in journals. There are variations in the way science is supported in different countries, and this is obviously reflected in the resulting possibilities for scientific research and achievements. It is one of the missions of the IUCr to stimulate the development of crystallography all over the world - in particular, in countries where there is limited funding.

The IUCr lends support to the development of crystallography in a variety of ways; visiting professorships that enable eminent scientists to participate in workshops and seminars held in developing countries, sponsorship of international meetings and grants that allow young scientists to attend international meetings. This support is a very important component of the activities of the IUCr and about \$150,000 is given yearly in support of meetings and young scientists.

You may have wondered how the worldwide economic crisis has affected the economy of the IUCr, and if it would have an impact on IUCr's support for crystallography. The economy of the IUCr is monitored carefully by the Finance Committee (www.iucr.org/iucr/index.html/finance.htm) through e-mail exchange and at two annual meetings. At a recent meeting (March 23-24) we had access to the almost final accounts for 2008.

The IUCr has three main sources of income, membership subscriptions, publications and returns from investments built up by income from journals since 1982 (90% of the total comes from publications). Publication of crystallographic journals was the driving force in the creation of the IUCr more than 60 years ago, and it is also the publishing activity of the IUCr (the eight journals and *International Tables*) that has provided the financial basis for the support of young scientists and international crystallographic meetings. Scientific publishing has undergone significant changes requiring major investments in the last 10 years, and in this period it was valuable to have income from the investments. The IUCr investments are held in the US (\$) and the UK (£), and in 2008 their value declined significantly. However, as the IUCr accounts are given in Swiss francs (IUCr is domiciled in Switzerland) and the Swiss franc strengthened in 2008 relative to the \$ and the £, this led to a further decrease of the value of the assets when expressed in Swiss francs. The good news from the 2008 accounts is that the publishing activity brought in sufficient money to enable the IUCr to operate with a small overall surplus so that there was no need to sell any assets to finance its activities. Some other good news is that ICSU (International Council for Science), of which IUCr is a member, has decided to base the dues from the scientific unions on the fees they receive from the members and not on the annual turnover (as originally proposed), which will almost halve the IUCr dues by 2012 to EUR 3500. If the turnover criterion had been employed, the dues of the IUCr would have increased by 500%. You can find details about the finances of the IUCr in the annual reports of the Executive Committee published as **open access** in *Acta Crystallographica* Section A; the report for 2007 was published recently [*Acta Cryst.* (2009) **A65** 52-75].

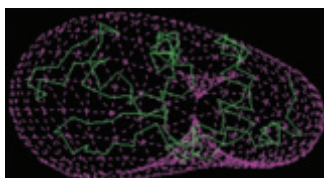
The Finance Committee concluded that it was important to continue the careful monitoring of the international financial situation and appreciated the small surplus provided by the publishing activity. This is therefore the time to express a great appreciation for all the people that contribute to the continued success of the IUCr publishing activity, namely the authors, editors and reviewers and, last but not least, the staff in Chester.

Sine Larsen (slarsen@esrf.eu)

IUCR JOURNALS NEWS

Molecular shapes from small-angle X-ray scattering: extension of the theory to higher scattering angles

***Acta Cryst.* (2009). A65, 128-134 [doi.org/10.1107/S0108767309003237]**



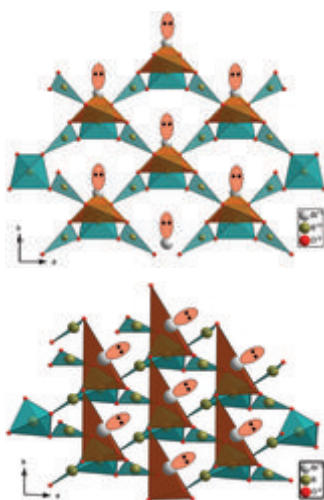
Molecular shape of lysozyme recovered from SAXS data up to $q=0.5\text{\AA}^{-1}$ (factor of 2π included). Coefficients of the multipole expansion of the shape of a dissolved molecule are related to measured small-angle X-ray scattering (SAXS) intensities, $I(q)$, through radial integrals with Bessel function kernels. These integrals are currently performed by analytical integrations of the individual terms of truncated power-series expansions of the Bessel functions, valid only for relatively low values of q . Performing these integrals analytically with entire Bessel function kernels, including a modeling of a molecular hydration shell, allows an extension of the theory to higher values of q .

V.L. Shneerson and D.K. Saldin

High-pressure crystal structure of the non-linear optical compound BiB₃O₆ from two-dimensional powder diffraction data

High-pressure crystal structure of the non-linear optical compound BiB₃O₆ from two-dimensional powder diffraction data

Acta Cryst. (2009). B65, 1-10 [doi.org/10.1107/S0108768108029340]



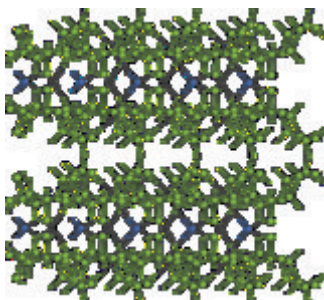
A method recently proposed by the authors for automatic detection, calibration and evaluation of Debye-Scherrer ellipses using pattern-recognition techniques and advanced signal filtering was applied to the 2D powder diffraction data of the non-ferroelectric, non-centrosymmetric non-linear optical compound α -BiB₃O₆ as a function of pressure. A non-linear compression behaviour over the entire pressure range is observed. At a pressure above 6.1 GPa, a first-order phase transition is observed, which is mainly characterized by a reorientation of the [BO₃]³⁻ triangles, the [BO₄]⁵⁻ tetrahedra and the lone electron pair which is localized at Bi³⁺, in order to optimize crystal packing (see figure).

R.E. Dinnebier, B. Hinrichsen, A. Lennie and M. Jansen

IUCR JOURNALS NEWS

The absolute configuration of 1-epialexine hemihydrate

***Acta Cryst.* (2008). C64, o649-o652 [doi.org/10.1107/S0108270108037086]**



Crystal packing in epialexine hemihydrate, showing hydrogen-bonding interactions which lead to the formation of a bilayered structure.

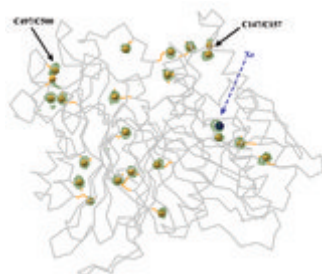
While determining the absolute and relative configuration of the natural product 1-epialexine, the Bijvoet pairs from data sets collected using both molybdenum and copper radiation were examined and compared using *CRYSTALS*. For the molybdenum data the Flack x parameter was refined to give an exceptionally large s.u. because there are no atoms heavier than oxygen. However, in contrast, the Hooft method suggests that the absolute configuration could be determined with a high confidence.

A.L. Thompson, D.J. Watkin, Z.A. Gal, L. Jones, J. Hollinshead, S.F. Jenkinson, G.W.J. Fleet and R.J. Nash

IUCR JOURNALS NEWS

De novo sulfur SAD phasing of the lysosomal 66.3 kDa protein from mouse

***Acta Cryst.* (2009). D65, 220-228 [doi.org/10.1107/S0907444908041814]**



Anomalous difference map contoured at 4.0σ (dark green). One peak represents the Xe atom, which is indicated as a blue sphere. For orientation, the C^α trace of the refined 66.3 kDa protein structure (PDB code 3FBX) is shown with cysteine and methionine side chains in stick mode and S atoms highlighted as yellow spheres. The two disulfide bonds are marked with black arrows.

The structure of the lysosomal 66.3 kDa protein from mouse has been determined by means of sulfur SAD (S-SAD) using crystals belonging to space group C2. Thus, this is one of the largest protein structures solved by S-SAD phasing so far and expands the limited number of successful S-SAD phase determinations in monoclinic space groups. The data exhibit an $R_{\text{anom}}/R_{\text{p.i.m.}}$ ratio of only 1.1. A single xenon atom caught in a hydrophobic pocket during a xenon soak was not required for successful phasing.

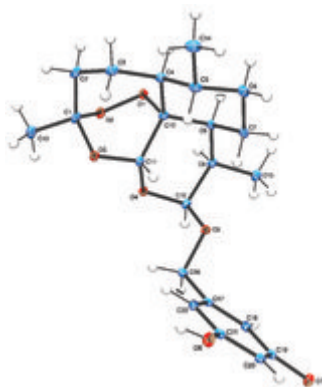
K. Lakomek, A. Dickmanns, U. Mueller, K. Kollmann, F. Deuschl, A. Berndt, T. Lübke and R. Ficner

IUCR JOURNALS NEWS

5- {[(3*R*,5*aS*,6*R*,8*aS*,9*R*,10*S*,12*R*,12*aR*)-3,6,9- Trimethylperhydro-3,12-epoxy-1,2- dioxepino[4,3-*i*]isochromen-10-yl]- oxymethyl}benzene-1,3-diol

5-{[(3*R*,5*aS*,6*R*,8*aS*,9*R*,10*S*,12*R*,12*aR*)-3,6,9-
Trimethylperhydro-3,12-epoxy-1,2-dioxepino[4,3-*i*]isochromen-10-
yl]-oxymethyl}benzene-1,3-diol

Acta Cryst. (2009). E65, o358-o359 [doi.org/10.1107/S1600536809002050]



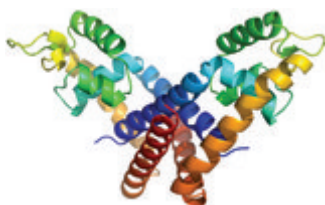
This dihydroartemisinin derivative is a fused five-ring system that has shown promising anticancer and antimalarial activity. The six-membered C_6 and C_5O rings display chair conformations. The six-membered trioxane ring has a distorted boat conformation with a C-O-O-C torsion angle of 42.55° for the peroxy group. The seven-membered ring C_6O has a distorted boat-type conformation, while the other (C_5O_2) has a distorted chair-type conformation. The structure contains intermolecular O-H...O hydrogen bonds linking the molecules into sheets parallel to the (100) planes.

W. Gul, P. Carvalho, A. Galal, M.A. Avery and M.A. El Sohly

IUCR JOURNALS NEWS

The structure of NMB1585, a MarR-family regulator from *Neisseria meningitidis*

***Acta Cryst.* (2009). F65, 204-209 [doi.org/10.1107/S174430910900414X]**



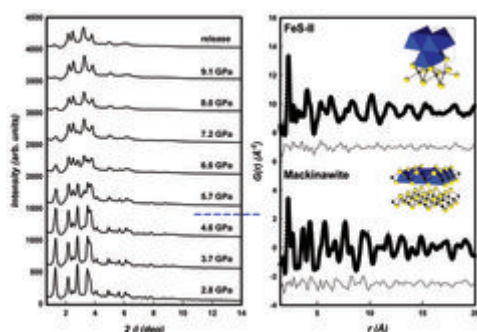
Members of the multi-antibiotic resistance repressor (MarR) family of transcription factors have been implicated in the control of multi-drug resistance in bacteria. These proteins regulate expression of transporter proteins by binding to specific sites in their gene promoters. We have solved the structure of the MarR protein NMB 1585 from the human pathogen *Neisseria meningitidis*. The structure resembles other MarR proteins comprising two wing-like DNA binding domains connected to extended α -helical arms which associate to form the protein dimer.

C.E. Nichols, S. Sainsbury, J. Ren, T.S. Walter, A. Verma, D.K. Stammers, N.J. Saunders and R.J. Owens

Structural changes in nanocrystalline mackinawite (FeS) at high pressure

J. Appl. Cryst. (2009). 42, 15-21 (doi.org/10.1107/S0021889808034730)

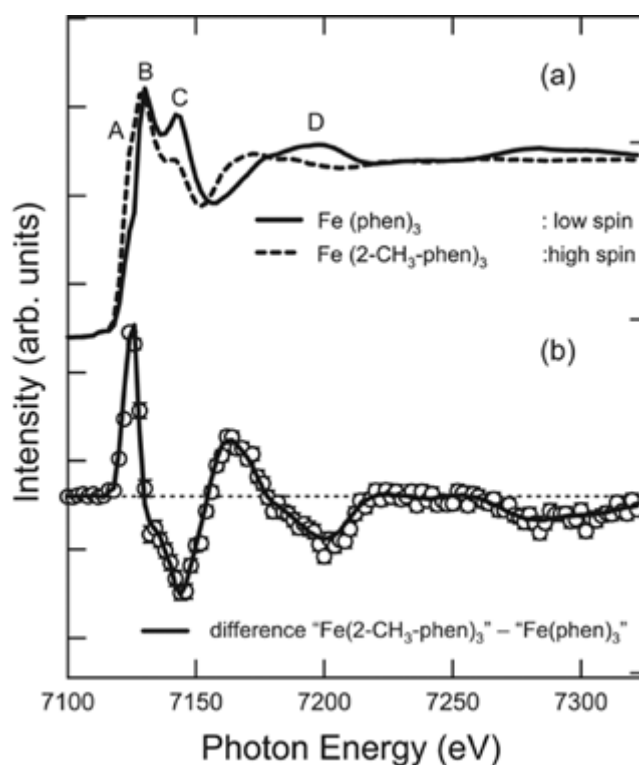
L. Ehm, F.M. Michel, S.M. Antao, C.D. Martin, P.L. Lee, S.D. Shastri, P.J. Chupas and J.B. Parise



The determination of the atomic arrangement in nanostructured materials is challenging. However, the atomic structure of nanocrystalline materials can be obtained using the atomic pair distribution function technique, which is derived from the Fourier transform of the total elastic X-ray scattering. The present article shows the successful structure refinement of nanocrystalline mackinawite at elevated pressure. A phase transition was observed and the structure of the high-pressure phase has been determined using a combination of model building and real-space structure refinement.

Capturing molecular structural dynamics by 100 ps time-resolved X-ray absorption spectroscopy

J. Synchrotron Rad. (2009). **16**, 110-115 [doi.org/10.1107/S0909049508034596]

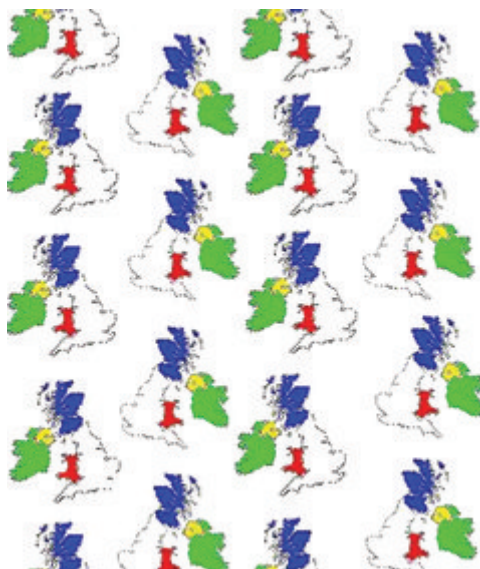


(a) Static and (b) photo-induced difference Fe K-edge TR-XAS of 50 mM $[\text{Fe}^{\text{II}}(\text{phen})_3]^{2+}$ in water. An experimental strategy and set-up for the 100-ps time-resolved X-ray absorption spectroscopy (TR-XAS) is presented. X-ray positional active feedback combined with a figure-of-merit scan of the laser beam position was employed as a key technique. It is shown that the pump-probe TR-XAS technique using the X-ray pulse structure at synchrotron sources is a powerful tool to investigate the dynamics of the electronic state and the molecular structure of non-crystalline samples. A TR-XAS measurement of a photo-induced spin crossover reaction of the tris(1,10-phenanthroline)iron(II) complex in water is presented.

T. Sato, S. Nozawa, K. Ichiyang, A. Tomita, M. Chollet, H. Ichikawa, H. Fujii, S. Adachi and S. Koshihara

SPECIAL REPORT

Crystallography in Great Britain and Ireland



The first question in writing about our little archipelago off the shores of northeastern Europe is what to call ourselves. The title chosen is, I hope, neutral and geographical, but willy nilly, the adjective 'British' will keep coming up to describe us all. It is to be understood in the same sense as the word 'European' in the European Crystallographic Association, which includes Africa! In any case, as the cover shows, the application of a little crystallographic symmetry can help us all fit together better!

These islands cannot claim to be the birthplace of X-ray diffraction, but we can lay claim to be the first home of crystal structure analysis, and, for our size, to have made very substantial contributions to the subject ever since. Most of this history is well known to crystallographers. A brief history of the formation of the British Crystallographic Association is included, but most of what follows here is an account of some of the work currently going on in universities and in industry. It is by no means complete, and I have left the style as it was contributed. In most cases, a large number of websites are not given - it is now usually easier to use a search engine to learn more of the work of a particular person or institution than it is to try to copy a website carefully from a printed page! We hope that you enjoy learning more about us!

Bob Gould for the British Crystallographic Association

Prehistory of the British Crystallographic Association



Although X-ray diffraction was founded in physics, it rapidly became an interdisciplinary subject. Its potential for discovering the arrangement of atoms in crystals was recognized by the British physicists William Henry Bragg and his son William Lawrence Bragg. Structural research was thus providing information that was fundamentally chemical. It was appropriate that W. H. Bragg's appointment to the Royal Institution in 1923 was not only as Director of the Davy Faraday Laboratory but also as Fullerian Professor of Chemistry.

The Royal Institution was able to play a key role in the interdisciplinary development of X-ray crystallography because it was not a university. In the 1920s, departmental divisions in universities between physics and chemistry were usually rigid. The crossing of subject boundaries at the Royal Institution was facilitated by a family atmosphere within the research team, attracting not only physics-trained graduates such as Kathleen Yardley (later Lonsdale) and Gordon Cox, but also chemists such as J. Monteath Robertson. These three all went on to head departments of chemistry in universities where they introduced crystallography as the main line of research. As a result, crystallography was broadened to include molecular geometry, intermolecular interactions, and the possibilities for chemical changes in the solid state, alongside the physical interactions between atoms and ions, and the physical characteristics of crystalline matter. Meanwhile, W.L. Bragg founded research schools in the physics departments at Manchester and Cambridge universities whose specialities included crystal structure determination of chemical materials alongside physical crystallography. He was also conscious of the important applications of crystallography in industry, and in 1942 he held a large conference in Cambridge on relevant topics. He then founded, in 1943, an X-ray Analysis Group (XRAG) within the Institute of Physics.

One of the first international X-ray diffraction meetings was organized by W.H. Bragg at the Faraday Society in 1929, and this laid the foundation of a more formal international collaboration between crystallographers. Committees were set up to introduce a coordinated abstract scheme, to standardize crystallographic nomenclature, and to prepare and standardize space group tables.

Publication of the first edition of the International Tables for Crystallography in 1935 was a major achievement, in which Kathleen Lonsdale played a particularly important part. The war severely hindered international cooperation in Europe, although in 1943, W.L. Bragg made a hazardous journey to Sweden to re-establish contact with Swedish scientists!

In postwar years, interdisciplinary collaboration in UK crystallography ran into some difficulty. In those years it was considered essential for a professional academic scientist to be a member of an appropriate society. The relevant societies for physics and chemistry were the Institute of Physics (IoP) and the Chemical Society (CS). In the 1950s, the IoP, having merged with the Physical Society, was not only a learned society, organizing and sponsoring scientific meetings: it was also a professional association, accrediting members at various levels, providing career advice and professional insurance, and publishing journals that were offered to members at a reduced price. The overhead costs of examinations, accreditation, publication, advisory services and insurance enforced a large annual subscription, equivalent to one or two weeks' salary for a young lecturer. The CS was the learned society predominantly serving academic chemists, accreditation functions being carried out by the then separate Royal Institute of Chemistry, and they did not merge until 1980. In universities, membership of the IoP or the CS conformed closely, in most cases, to departmental boundaries between physics and chemistry.

Originally, XRAG provided a valued meeting point. Because chemical crystallographers had no corresponding group, many chemists joined the IoP at the cheapest grade of Subscriber and could take part in XRAG with no additional payment. XRAG meetings catered to the interests of physical, chemical and biological crystallographers, and to some extent those of mineralogists, geologists and metallurgists.

This amicable state of affairs continued until 1966. By that time the volume of research in chemical crystallography had grown to such an extent that it was felt there should be a Chemical Crystallography Group (CCG) of the CS. Under the chairmanship of Monteath Robertson, the new Group encouraged more activity among chemists in using the techniques and results of structure determination. Though this was a useful development, it caused some ill feeling, because it created a separation between physical and chemical crystallographers, when a single group had been so successful in the past. Some chemists continued to belong also to XRAG, which in 1969 became the Crystallography Group of the IoP (here called PCG to avoid ambiguity!). Without anybody wishing it, the barely significant difference between

physical crystallographers and chemical crystallographers had been set in stone because of the rigid walls between physics and chemistry departments in many universities.

On the initiative of the PCG committee, under the chairmanship of Ted Steward, a United Kingdom Crystallographic Council (UKCC) was set up in 1969 which tried to prevent overlaps between crystallographic meetings, both of dates and topics, and to encourage occasional joint meetings. It catered not only to chemists and physicists but also to other crystallographers. It fulfilled a useful function, but because it had to avoid challenging the roles of the PCG and the CCG it proved too weak and ineffective to become a unifying British crystallographic society. It was the establishment of the European Crystallography Meeting (now the ECA) in 1970, and discussions about how the UK should be represented on it, that brought the groups together, with a joint members' meeting in 1971.

Meantime, the Royal Society had set up the British National Committee for Crystallography (BNCC) to represent it on the IUCr and to distribute its block grant for scientists attending the meetings of the IUCr. This job was complicated by the division in British Crystallography, and in 1978, Arthur Wilson, then chairman of the BNCC, proposed that it should provide an umbrella organization for the CG, the CCG and the UKCC. An ad hoc group was established, and it prepared a proposal for the 'Formation of a British Crystallographic Association' which was presented by Andrzej Skapski to the BNCC in May, 1979. However, there were two main difficulties - financial and organizational. The report said: 'A reserve fund of £4000-5000 would be invaluable in aiding the BCA to start its activities.' And was it right to attract membership from crystallographers loyal to the existing groups?

In the summer of 1980, John Robertson, in an article published jointly in the PCG and CCG newsletters, said that 'the crystallographic community of this country is divided into two major portions; there is consequent loss of much of the richness of our subject, and consequent frustration for our committees.' This alerted the two groups to the seriousness of the division but it was Stephen Wallwork who suggested how it might be overcome. His idea was that the PCG and CCG members should automatically belong to the new organization and these groups should continue unchanged, as joint groups linked both to their own society and to the new organization.

Important steps were taken at the J. M. Robertson Symposium held in Glasgow in September 1980, a landmark meeting because it included the two groups. Wallwork's proposals were favourably discussed and it was decided to arrange a special meeting of the two groups to consider them in more detail and, if they were accepted, to set up a working party to plan the formation of the new body. The initial proposals were put to the Councils of the RSC and the IoP, who were both very supportive. The Working Party rapidly agreed the name 'British Crystallographic Association' (BCA) and began work on a draft constitution. Wilson, who had much experience of this kind of drafting, was the mastermind in this activity. In comparison with the UKCC, the new organization would be much more powerfully placed to be the national representative of UK crystallography. The working party also set a target date for inauguration of the BCA at a crystallographic meeting in Durham, already planned for April 1982, a target that maintained a sense of urgency.



At the historic meeting in Durham, 1982, left to right: Brian Isherwood, Arthur Wilson, Andrzej Skapski, Charles Taylor, David Blow and David Phillips

A proposal made in May 1979 to amalgamate the two newsletters was finally implemented, and in March 1981 the first joint issue of a newsletter, edited by Moreton Moore, was published by the PCG and the

CCG. The second issue (June 1981) was entitled *Crystallography News*, and it is still published under this name.

After considerable delay, approval of the charitable status of the new organization was obtained only three weeks before the inauguration date. David Blow had solved the problem of initial financial resources by suggesting that crystallographers should be invited to become founder members. By the inauguration date, 23 of these had guaranteed £100 each (as a ten-year membership subscription) and there were also five founder sponsors at this stage, offering £1850. The Inaugural Meeting on April 6, 1982, was attended by 127 people, and the recommendations of the working party were accepted unanimously, including the election of Sir David Phillips as President, and Dorothy Hodgkin as Vice-President. Hodgkin and Henry Lipson spoke at the inauguration. At the end of the inaugural meeting, Brian Isherwood proposed the establishment of an Industrial Group of the BCA, and David Blow proposed the establishment of a Biological Structures Group. This structure of four specialist groups within the BCA still survives, the Crystallography Group of the IoP having become the Physical Crystallography Group.

At the end of this historic meeting there was a great sense of euphoria. At the same time, members of the working party were well aware that the financial resources of BCA were inadequate. Indeed, some even doubted whether it could survive. The financial position soon improved, however, helped by the founder schemes. These were held open until the end of 1982, after which there were 52 Founder Members, and also 31 Founder Sponsors who donated over £12,000 between them. Most importantly of all, the BCA succeeded beyond all expectations as a scientific organization, with its active groups, its exciting annual meetings and, crucially, its large and enthusiastic membership. It has become one of the biggest crystallographic societies in the world.

David Blow and Stephen Wallwork

[Reprinted from *Crystallography News* 98, (2006). A fuller account is published in *Notes Rec. R. Soc. Lond.* **58**(2), 177-186(2004)]

Current BCA officers



From left to right: President: Elspeth Garman, Vice president: Alexander J. Blake, Secretary: Georgina Rosair, Treasurer: Harry Powell.

Central facilities in the UK

The IUCr in Chester



Although the IUCr is domiciled in Switzerland, all its administrative and publishing activities are carried out from its offices in Chester, UK. By 1962 the technical editing workload for the Union's publications had become too heavy for the university workers who had been doing this on an honorary basis since

1948. Thus, Stephen Bryant was appointed as the Union's first full-time Technical Editor; Stephen lived in Chester (he had previously been Senior Technical Editor at Shell's Thornton Research Centre near Chester). The first Union office was a room in Stephen's house!



IUCr stand at a BCA meeting: Andrea Sharpe with Bill Clegg.

The Union's first Executive Secretary, Jim King, was appointed in 1968 and the Union's joint administrative and editorial office was formed. Since those early times, the number of staff has increased as the size, scope and number of journals and other publications, such as the *International Tables for Crystallography*, has grown, and the office has moved to various locations within Chester to accommodate the increase. The Union now occupies three of the buildings in Abbey Square, and has three staff working in administration, 11 carrying out editorial work, four in R&D and one in promotions. The staff work with 39 Adhering Bodies and 19 Commissions; in addition, the publishing operation involves cooperation with over 150 scientific Editors and Co-editors worldwide and produces approximately 4000 papers and 15000 pages each year.

Just as computers and the internet have played a large part in crystallography they have also been important in crystallographic publishing in Chester. The work carried out has changed enormously, in line with the rapid developments in the printing industry and computing. Whereas in the past, journals were submitted as paper manuscripts and typeset using metal type, IUCr publications are now typeset electronically from files submitted online by the authors, and printed by 'direct to plate' methods.

The growth of the internet has meant that more publications are available online and the IUCr in Chester has been at the forefront of these developments. All the IUCr journals from 1948 to present day are available via Crystallography Journals Online (journals.iucr.org) and all eight volumes of the *International Tables* are available via *International Tables Online* (it.iucr.org).

The staff in Chester have worked closely with the crystallographic community on standards for the publication and interchange of crystallographic data. The work on the development of CIF, recognised in 2006 by the prestigious ALPSP Award for Publishing Innovation, has been a great success and has transformed the way small-molecule structural papers have been handled and data transferred to the databases. For macromolecules, it is envisaged that work in progress on mmCIF will facilitate transfer of data between authors, databases and journals in a similar way.

The IUCr operations are thus a small but important part of Crystallography in the UK. The IUCr staff would like to thank all those worldwide who have helped with their time and effort in making the work of the organization a success.

Andrea Sharpe

CCP4



The 'Collaborative Computational Projects' or CCPs in their heyday ran up into the teens. By far the hardest has been CCP4, whose influence has been very great worldwide.

CCP4 is undoubtedly the most successful of the collaborative computing projects begun in the 1970s. For some reason, the name always makes me think of it as an organisation emanating from the cold-war era USSR, and to a certain extent it has been run along true socialist lines. The aim of CCP4 is to provide distribution of, and support for, software contributed by developers to whom no funds return directly. Rather, the developers receive funding from granting bodies, which expect the work to be made easily and quickly available to other crystallographers (whom the same funding bodies also support), a win-win situation. Traditionally, the rather gulag-sounding Working Groups 1 and 2 have run CCP4. Any PI in the UK can vote in the decisions of Working Group 1, which sets general policy, and any crystallographer in the UK can join CCP4 Working Group 2, which liaises between users and developers. More recently CCP4 has acquired an Executive and a Scientific and Technical Advisory Board (STAB) to give more direction to the expanding team of scientists associated with CCP4. The nature of CCP4 has meant a constantly changing cast of contributing characters in the various working groups, Executive and STAB, so CCP4 has been fortunate to have had the guiding influence of Phil Evans and Eleanor Dodson since its inception. CCP4 has also had long-term financial and legal underpinning from CCLRC, and is currently funded by a grant from the BBSRC.

CCP4 faces one enormous opportunity and one enormous challenge in the years to come. The opportunity comes from the imminent move of the CCP4 group from Daresbury to Diamond and the challenge comes from the increasing desire of universities and funding bodies to financially exploit the commercial potential of software.



CCP4 people at Daresbury CCLRC Back row L-R: Francois Remacle, Charles Ballard, Dan Rolfe; Front row L-R: Maeri Howard, Peter Briggs, Martyn Winn, Norman Stein, Wanjuan Yang; Missing: Ronan Keegan. The move of CCP4's home from Daresbury to Diamond will give wonderful opportunities to collaborate with the beam-line scientists there and contribute to the development of streamlined structure solution pipelines. CCP4 will also benefit from being close to the new epicentre of practical macromolecular crystallography in the UK, and the regular visits from international scientists attracted by the state-of-the-art facilities. CCP4's years of accumulated experience in maintaining and distributing software over many software aeons (an aeon being about three years!) will also benefit other groups working at Diamond. This should be a well-funded enterprise, as structural genomics is seeing a large injection of funds into the development of software for structural biology. CCP4's has already collaborated with the SPINE, BIOXHIT, eHTPX and MAX-INF initiatives.

On the flip-side, the changing environment for the commercialisation of university research is a factor that CCP4 needs to adjust to. CCP4 has relied on licensing software from contributing developers without providing financial recompense. In the very beginning this arrangement was not even formalised, but mostly has been the subject of a contract made directly between the developer and CCP4 through CCLRC. Unfortunately, this direct relationship is being eroded by the increasing desire of institutions and funding bodies to stake a financial claim. Software is an attractive target for this interest, because it is directly saleable: it does not have the lead-time required to reap royalties from products that require manufacture. Another issue concerns the increase in litigation, which means that organisations are becoming more pro-active in their desire to limit their liability in case of software errors. Although it is exceptionally difficult to think of a scenario in which CCP4 software could be at fault to this degree, this

issue has been the subject of a protracted dispute over the terms of the license under which future versions of CCP4 will be distributed, and the issue is currently unresolved. Despite these problems, CCP4 has recently attracted high-quality and popular new software programs to the suite. Together with in-house software developments, these keep CCP4 at the forefront of crystallographic methods development.

CCP4's contribution to macromolecular crystallography is not confined to the distribution of the CCP4 suite. CCP4 reaches out to the crystallographic community by attending most international crystallography meetings. The CCP4 Bulletin Board provides a lively forum for discussions on a wide range of protein crystallography topics, and CCP4 also produces a biannual newsletter that contains articles of general interest to crystallographers. The annual study weekends (held in early January each year) are a fixture of the crystallographic calendar and are a unique opportunity for developers to come together and discuss their latest ideas in focussed areas, such as molecular replacement, the topic of the 2007 Study Weekend. The goodwill that such activities generate in the crystallographic community will undoubtedly help CCP4 survive and thrive through its challenges.

Airlie McCoy

Particular thanks to Phil Evans and Martyn Winn for clarification of some details in this article.

Crystallography at the Synchrotron Radiation Source, Daresbury Laboratory



Crystallography was well represented at the SRS from the start of user operations in 1981 and remained a key activity until the last photons were delivered in August 2008. So much has been achieved that a short article cannot possibly do it justice: this overview will briefly highlight some of the major successes and developments over the years but, inevitably, many important advances will be omitted (see <http://www.srs.ac.uk/srs> for more detail). From the outset X-ray beamlines on the SRS provided instruments for protein crystallography (PX), fibre diffraction and topography, and within a few years the first superconducting wavelength shifter was delivering intense photon beams for high resolution powder diffraction (HRPD) and surface crystallography. X-ray absorption spectroscopy (XAS), which provides local structural detail and valence state information to complement crystallographic parameters, and small angle X-ray scattering (SAXS) techniques were also available and, like PX, the demand for these grew significantly justifying the construction of further beamlines.

Many advances were achieved through developments in detectors, data acquisition systems, focusing X-ray optics, and sample chambers (one for *in situ* molecular beam epitaxy perhaps being the most complex). For example, instruments built by the Daresbury Laboratory's Detector Group led to and helped retain the SRS's competitive edge by efficiently recording photons in both one and two-dimensions leading to information on chemical composition, as well as structure and kinetics under rapidly changing conditions. Similarly, the Collaborative Computational Projects (CCPs) developed data analysis methods in parallel and these continue to act as central repositories and suppliers of software to the community world-wide for PX, XAS, SAXS, powder and single crystal diffraction.



Aerial view of Daresbury Laboratory

The PX beamlines were upgraded many times and witnessed truly massive advances from the early days of multi-pack film exposures to 'tiled' CCD detectors leading to fast data collection and 'same-day' structure solution. It was exceptionally rewarding that the SRS played a part in John Walker's 1997 Nobel Prize in Chemistry *for elucidating the enzymatic mechanism underlying the synthesis of adenosine triphosphate*. There has been a broad impact on molecular biology from other beamlines too, such as SAXS beamlines (through studies of DNA and muscle) which are now more commonly used for solution scattering experiments to gain details of molecular shape, particle size and nucleation, and for studying crystallinity in polymers. Early applications of circular dichroism to protein folding studies led to a dedicated beamline being built to study such mechanisms. The most recent PX beamlines largely used high flux multipole wiggler sources and state-of-the-art ADSC Quantum detectors. Wavelength selectivity (to optimise and exploit changes in f' and f'') is of course a fundamental reason for using synchrotron radiation (SR), and latterly PX routinely exploited this on the SRS. High throughput was achieved by robotic systems taking cryo-cooled crystals from storage racks, mounting, centering, and replacing them after data collection: in this way, crystal screening identified the best diffracting sample for subsequent full data collection. Apparatus was also developed to enhance crystallinity by varying humidity around the protein and then a microfocus beam was used to investigate ever smaller crystals (so requiring less starting material).

The launch of small molecule crystallography (SMX) on the SRS was an immediate success. For the first time, a dedicated, tuneable-wavelength beamline permitted structure solution using crystals too small and/or too weakly diffracting to be studied on conventional sources. This beamline was always heavily oversubscribed and highly productive, having delivered over 500 publications in 10 years, and a second, fixed-wavelength beamline was eventually built to increase capacity and provide beamtime for technique development. By then, both beamlines had Bruker ApexII detectors which, combined with the high flux, could record a full sphere of data in less than an hour. The last three years saw a growing emphasis on *in situ* experiments on single crystals to follow structural changes resulting from variations in physical or chemical conditions. Temperature was controlled simply using nitrogen or helium gas streams (10 K to 750 K) or a 'hot-head' goniometer, and pressure was varied using diamond anvil cells (DACs). Another sample cell (designed and built in-house) surrounded the crystal in different gaseous environments e.g. to allow the exchange of molecules inside nanoporous structures to be studied in detail. In common with research at other synchrotrons, significant progress was made with techniques to investigate molecules in transient excited states - termed 'photocrystallography' - and fascinating, and often unexpected, results were obtained. Both beamlines were accessed by the EPSRC-funded National Crystallography Service to examine crystals that resist structure solution on laboratory diffractometers using conventional X-ray sources.

Twenty years of powder diffraction on the SRS's high flux beamlines contributed to landmark results in fundamental physics and chemistry, pharmacy, engineering, magnetism, and Earth and environmental science. Variable temperature (80 K to 1250 K) was a common requirement but a much larger range of *in situ* experiments was tackled on the SRS. Energy-dispersive powder diffraction (EDPD) was used for experiments on samples contained in vessels with steel walls or restrictive X-ray windows. For example,

a large volume hydraulic press, housing minerals in 1 cm³ capsules, simulated the high pressures and temperatures deep in the Earth. EDPD was also used for strain scanning of large engineering components constructed from steel or aluminium alloy such as aircraft components where tensile stresses might lead to catastrophic failure. A multipole wiggler beamline used mirror and sagittal crystal focusing to deliver very high flux monochromatic radiation for materials processing investigations: high count-rate RAPID detectors developed at Daresbury Laboratory recorded both wide- and small-angle scattering. Powder diffraction was combined with XAS and SAXS techniques on other beamlines too, for which a wide angle gas-microstrip position sensitive detector (HOTWAX) was developed in-house.

The crystallographic study of matter at high pressure in DACs was revolutionised following the introduction of image-plates in the early 1990s. Many structures previously recorded by EDPD methods were found to be incomplete or wrong. Systematic monochromatic studies of the elements and binary systems, some of which exploited resonant scattering, revealed both simple and highly complex structures. More recently, a flux gain of over 50 achieved with focusing Laue optics, when combined with an *in situ* read MAR345 image-plate, drastically reduced the rate limiting steps of recording and extracting the digitised data opening up a wealth of new possibilities across a broad range of science. This cutting edge research contributed to world leading advances such as structure solution from single crystals grown under pressure within the DACs from the powders of newly identified high-pressure polymorphs.

The SRS clearly made some important contributions to crystallography in industry in the UK (and in several other countries) through *DARTS* - see <http://www.darts.ac.uk/> - by making a broad range of SR techniques available to organisations and offering a full materials characterisation service to businesses that did not have in-house crystallographers. This pioneering approach provided industries with data unobtainable from conventional X-ray sources (i.e. better spatial or time resolution, better signal to noise ratio, a combination of *in situ* measurements etc.) that proved to be critical to solving specific problems or making advances having short- and long-term commercial impact.

User operations on the new UK synchrotron, Diamond, began last year and the SRS has now 'handed over the baton' along with the legacy of thriving communities eager to undertake imaginative experiments to exploit the brighter photon beams. Crystallography will again be well represented and results are already showing that this new source, designed at Daresbury Laboratory, can meet the ever increasing demands placed on such facilities and allow UK users to compete on the world stage well into the future.

Graham Bushnell-Wye

Crystallography on the Harwell Science and Innovation Campus

This campus is in Oxfordshire about 15 miles south of the city of Oxford, in a rural area of the North Wessex Downs designated as an 'Area of Outstanding Natural Beauty' with good road and rail connections and about an hour's drive from Heathrow airport. User accommodation is available on campus. Two of the laboratories on this site are described below, the Rutherford Appleton Laboratory and the Diamond Light Source.

The Rutherford Appleton Laboratory

This multi-disciplinary laboratory maintains a proton synchrotron originally built for particle physics research in the 1960s. After the creation of the Centre for Research in Nuclear Physics (CERN) in Geneva, particle physics experiments moved to CERN and this synchrotron was converted into a spallation neutron source by extracting the proton beam on to a target to produce pulsed neutrons. At this time it

was renamed ISIS. Moderators and choppers are used to produce beams of several different energies depending on the science to be studied and the instrument with which they are to be used.

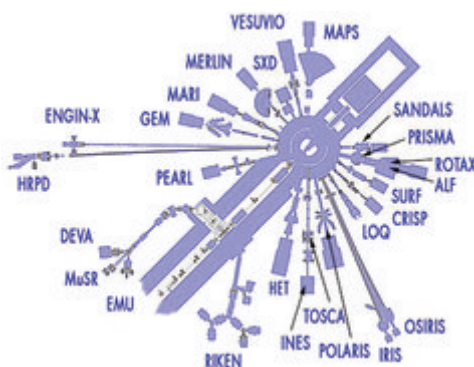


Figure 1

Neutrons are particularly good for studying the positions of hydrogen atoms which are more difficult to see using X-rays and since they have spin they can be used to study magnetic structures. The pulsed nature of the source means that time-resolved studies of changing structures can be carried out here. The facility provides beams of neutrons and other particles, muons, that enable scientists to probe the microscopic structure and dynamics of matter in areas encompassing physics, chemistry, earth science, materials science, engineering and biology. Altogether there are now 24 instruments, each with web pages of information on the instrument characteristics and applications. They are grouped together by scientific interest, for example, the crystallographic instruments are GEM, HRPD, PEARL, POLARIS, ROTAX and SXD while that for engineering applications, such as measuring the strain in railway lines, uses ENGIN-X. Further web pages provide summaries of each instrument suite to help you decide which instrument at ISIS could be suitable for your experiment.

The diagram (Fig 1) shows the clustering of the instruments around the target station in the experimental hall. The muon instruments, DIVA, MuSR and EMU are attached to one side of the extracted beam on the lower left, RIKEN on the other side.

Details can be found on the ISIS website at www.isis.rl.ac.uk/.

Reports on the recent science performed at ISIS can also be found there. Plans for a European spallation source are still on the drawing board so ISIS will remain Europe's only source of pulsed neutrons for the next few years.

The ISIS Second Target Station project

The accelerator can produce more protons for a second target station which will allow more instruments to be used and the ISIS program to expand into the key research areas of soft matter, advanced materials and bio-science providing 'cold' long wavelength neutrons with energies from 5×10^{-5} to 0.025 eV. Construction of the second neutron source began in July 2003; first neutrons have been produced. When the experimental program begins, seven new state-of-the-art instruments will be available to use the high flux of long-wavelength, low-energy neutrons. There are plans for a total of eighteen instruments which will involve scientific input from researchers in more than 10 countries around the world. Live web cameras show the progress of construction at <http://ts-2.isis.rl.ac.uk>.

There is not room in this article to describe all the instruments, so I mention just the one which provides high-resolution magnetic diffraction. The ability to produce diffraction patterns at nearly constant resolution over a wide range of lattice-spacings is one of the distinct features of time-of-flight sources such as ISIS. WISH is a long-wavelength instrument optimised for studying magnetism at an atomic level.

Designed for powder diffraction at long d -spacing in magnetic and large unit-cell systems, it will specialise in such topics as magnetic clusters and extreme conditions of magnetic field and pressure.

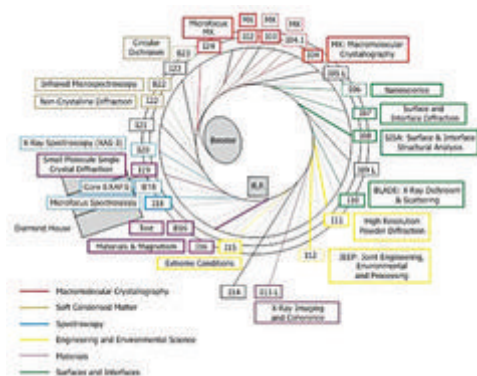
Diamond Light Source (DLS)

The UK Government, via the Science and Technology Facilities Council (STFC), formerly the Central Council Laboratory of the Research Councils (CCLRC), and the Wellcome Trust sealed their partnership to build and operate the Diamond synchrotron on March 27, 2002. A joint venture company, Diamond Light Source Ltd, was then established to run this mission led by its Chief Executive, Gerhard Materlik.

The company is owned by its shareholders: STFC own 86%, the Wellcome Trust 14%. Other parties can buy shares in the company with unanimous agreement of the existing shareholders. The funders have committed to construct, commission, operate and decommission the Phase I facility consisting of the core facility, an electron synchrotron and seven beamlines and their associated instrumentation. Phase II, a further 15 beamlines, will be added at a rate of four or five per annum. Phase III will depend on user requirements as the facility develops. There is also the potential for User Installed Beamlines similar to the Collaborative Research Groups (CRGs) at the European Synchrotron Radiation Facility (ESRF).

Beamtime is allocated on the principle that it is funded by third parties to be provided free at the point of use to all academic and scientific users. Allocation is via a peer review process, operated by DLS to select proposals on the basis of scientific merit. A minimum of 30% of the time is made available for academic and charitable life sciences research.

In line with other synchrotrons, there are opportunities for third parties to use the facility, either by constructing their own beamlines or by purchasing beamtime. Any income raised through user charges are to be used to offset the facility operating costs or held as a contribution towards the costs of decommissioning the facility.



Diamond is a third-generation 3 GeV (Giga electron Volt) synchrotron light source. Third generation light sources use arrays of magnets, called insertion devices, to generate extremely intense, narrow beams of electromagnetic light, about 10,000 times brighter than the UK facility based at the Daresbury Laboratory in Cheshire. Diamond is currently the best medium-energy X-ray source in the world; it is optimised to produce X-rays with energies between 100 electron volts (soft X-rays) and 20,000 electron volts (hard X-rays). In addition, Diamond also provides a good source of X-rays up to 100,000 electron volts.

A series of pages on this website describe case studies of industrial applications by sector, including aerospace, automotive, bioscience, electronics, IT hardware, engineering, environmental science and studies to improve how ingredients in food products behave at the molecular level during manufacture. It has facilities to study both the very small, for example viruses and the drugs needed to combat them, and the very large such as airplane parts.

The seven beamlines of Phase I are now in operation, a further 22 should be available by 2012 and there is space for more.

Full details can be found at www.diamond.ac.uk/ where there is a clickable map of the beamlines confirmed to date covering the first five years of operation.

The UK Prime Minister visited Diamond in November 2006 to celebrate first light in the beamlines. In February 2007 the first scientific user was welcomed on beamline I06, many more have done experiments since then.

Kate Crennell

Acknowledgement: Most of the material in this article has been extracted from the websites provided by the laboratories. Please look at these websites for more complete current information than I have been able to summarise here.

STFC UK Science and Technology Facilities Council: www.stfc.ac.uk/

ISIS spallation neutron source: www.isis.rl.ac.uk/

ISIS 2nd target station: <http://ts-2.isis.rl.ac.uk>

DLS: www.diamond.ac.uk/

The UK National Crystallography Service (1981-...)

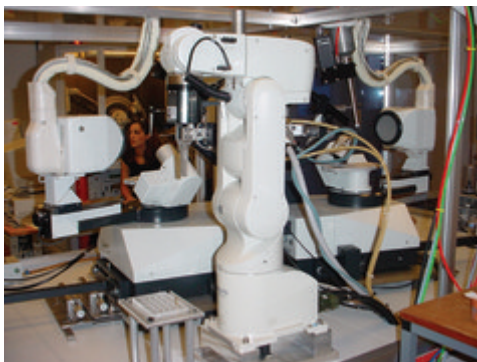


NCS staff, left to right: David Hughes, Thomas Gelbrich, Mike Hursthouse, Simon Coles and Peter Horton. When the current funding period expires (Oct. 2009) the EPSRC UK National Crystallography Service will celebrate 28 years of continuous operation.

Under the directorship of Mike Hursthouse and funded by the chemistry program of the UK Research Council in its various guises - SRC, SERC, EPSRC, the Service was formally instituted in 1981 at Queen Mary College, London. For a number of years, the Service relied on a PDP8-controlled CAD4 diffractometer, which had previously been funded to support collaborations between the QMC crystallography group and a small number of external users. New users were quick to seek access to the Service, and the load was quite a handful for the one RA staff member, Anita Galas. As demand increased, additional staff members were appointed, and the Service also instigated new directions in computing habits. In the 1982 renewal, funds were awarded to purchase a dedicated 'main-frame' computer - a VAX 11/750. In 1988 this machine was retired when the move was made to a PC-based computing environment, with four 286 PC's hosting T800 transputers. Each of these was more powerful than the VAX, and the cluster was purchased using two years' worth of VAX maintenance contract money!

With such an active user base, there was no shortage of samples and the datasets, structures and publications flowed copiously. Spurred on by the obvious demand, Mike turned his attention to searching for new technology for faster data collection and obtained additional funding at the time of the 1988 renewal to develop area detector technologies for small molecule crystallography. By 1990 the National Service was producing crystal structures at an unprecedented rate using a Nonius FAST TV area detector. The success of this technology catalysed the current day CCD revolution. The staggering rate at which

structures were being generated was also helped by the unique rotating anode source equipped with a molybdenum target. By 1997 it was time to embrace CCD technology and the throughput of the Service was intensified by coupling such a detector with a new Mo rotating anode.



The use of a highly sensitive detector operating in thick slicing mode with a new, state-of-the-art high flux RA generator, and new data processing and refinement software from the instrument manufacturers and academic colleagues, enabled the Service to tackle crystals that were so small or poorly formed that they would have previously been thrown away! Heading into the new millennium saw the Service, now based at the University of Southampton, as one of the most productive small-molecule crystallography facilities in the world.

Funding awarded in 2001 saw the addition of a second Kappa CCD to the rotating anode. At the same time, the Service commissioned the design and build of revolutionary X-ray focussing mirrors for Mo radiation which produced another giant leap forward, increasing the intensity of the source by a factor of six! In the laboratory, the Service could now handle exceptionally small crystals, mere microns in size, which would have previously required access to a synchrotron! However our users continue to test us with smaller and more demanding crystals and this renewal also saw the introduction of the synchrotron component of the National Service, which is run in collaboration with W. Clegg (Newcastle). The Southampton operation ensures that only the most suitable samples are sent to the synchrotron, where the service has approximately 40 days beamtime split evenly throughout the year.

The Service currently handles around 1200 samples a year, and, together with in-house work, the Southampton laboratory produces in excess of 2000 datasets and directly publishes over 70 papers per annum. Many additional publications are added to this total by Service users. In 2002 the Service became heavily involved in an e-Science pilot project. This has resulted in the development of an internet-mediated service which allows users to monitor the progress of their samples through the system, interact with the data collection and download their data. We are also pioneering the application of further automation in hardware and software in small molecule crystallography, starting with robotic handling of sample mounting, through data collection and processing, structure solving and validation to public dissemination. A highly successful pilot project around electronic data publishing has resulted in the eCrystals software, which is now being made available to the community. We hope this will provide a more open service to our users and a large increase in the provision of structural data to the chemistry community.

Simon Coles & Mike Hursthouse.

Southeastern England

Crystallography in London

Biological research



Research activities within structural biology across London are coordinated by the London Structural Biology Consortium, created in October 2002. All academic structural biology research groupings are represented: Birkbeck, Cancer Research UK, Imperial College, Institute of Cancer Research, King's College, National Institute for Medical Research, Queen Mary, School of Pharmacy and University College. The School of Crystallography at Birkbeck concentrates on structural biology, biophysics and bioinformatics as part of the Birkbeck/UCL Institute of Structural Molecular Biology. The School's approach to structural biology is increasingly one of combining protein crystallography with single-particle cryo-electron microscopy and 3-D reconstruction. There is a focus on pathogenesis and bacterial toxins (Gabriel Waksman, David Moss, Bonnie Wallace, Helen Saibil, Nicholas Keep), cancer and DNA repair (Neil McDonald, Tracey Barrett, Elena Orlova), chaperones, protein folding diseases and cataract (Helen Saibil, Elena Orlova, Nicholas Keep, Bibek Gooptu, Christine Slingsby) and cytoskeletal structure and function (Carolyn Moores, Nicholas Keep).

The Cancer Research UK London Research Institute operates at two locations. At the Clare Hall Laboratories, the research of Dale Wigley is focused on the enzymes that are involved in the replication and repair of DNA, utilising a variety of techniques in molecular biology, enzymology and X-ray crystallography. At the Lincoln's Inn Fields Laboratories, one long-term research goal is to understand protein regulation in the brain, including implications for neurodegeneration and cell-cycle control (Helen Walden). There is also interest in determining the structures of some of the multi-protein complexes that comprise the kinetochore (Martin Singleton), particularly those proteins involved in binding centromeric DNA and the complexes implicated in generating the spindle checkpoint signal at the kinetochore.

The Imperial College Centre for Structural Biology comprises over 20 affiliated research groups within the divisions of Molecular Biosciences and Biology, School of Medicine and Dept. of Chemistry. A major research theme is the development of new techniques for crystallization and crystallography of membrane proteins (So Iwata, Naomi Chayen), which has led to creation of The Membrane Protein Laboratory (MPL) as a joint venture between Imperial College and the Diamond Light Source, funded by the Wellcome Trust. The facility, under the directorship of So Iwata, is housed in a laboratory next to the beamlines at Diamond and became available for users in January 2008. The MPL is designed to train users in membrane protein crystallization and is also involved with the development of new methods for crystallization and data collection on membrane proteins, in collaboration with Gwyndaf Evans at Diamond. Members of the MPL are involved specifically in crystallization and structure determination work on a number of membrane proteins from the transporter, ATPase, respiration and GPCR families. Structural research at the Centre has included determination of a number of important crystal structures, including the human DNA repair enzyme Ape-1, XRCC1 BRCT domain, porcine spasmodic polypeptide,

and the disease-associated ATPase p97 (Paul Freemont). The Centre also has biomolecular NMR facilities (Stephen Matthews) and bioinformatics research (Michael Sternberg).

In the structural biology group at The Institute of Cancer Research, techniques of X-ray crystallography, electron microscopy, biophysics, biochemistry and molecular biology are combined to understand the structural basis for the function and regulation of proteins and complexes implicated in cancer. Research programs cover a range of key molecular systems and processes, including signal transduction (David Barford, Laurence Pearl, Richard Bayliss), cell-cycle control (Barford), transcriptional regulation (Pearl, Jon Wilson), targeted protein destruction (Barford, Ed Morris), chaperone function (Pearl), DNA repair (Pearl), chromatin modification (Pearl, Wilson) and chromosome dynamics (Bayliss). In addition to basic science programs, the section maintains close links with other groups that are involved in developing new therapeutics targeted at these systems, both within and outside The Institute of Cancer Research.

As part of the Randall Division of Molecular & Cell Biophysics at King's College London, the research interests of the structural biology group include structural studies on oxygenases (Roberto Steiner), antibodies that mediate allergy and asthma (Brian Sutton, Andrew Beavil), enzymes responsible for bacterial resistance to antibiotics (Paul Brown), protein/RNA complexes involved in RNA metabolism and initiation of translation (Sasi Conte), enzyme complexes that recognise and repair damaged DNA (Mark Sanderson), and proteins involved in the polyglutamine expansion diseases and other neurodegenerative disorders (Yu Wai Chen). A structural bioinformatics group has been established (Franca Fraternali) with research interests in the analysis and prediction of protein/protein and protein/nucleic acid interactions, and the analysis of small molecule/macromolecule interactions.

At the MRC-National Institute for Medical Research (NIMR) the structural biology group employs crystallography as one of a wide range of biochemical and biophysical techniques, including electron microscopy, NMR spectroscopy and single-molecule measurements. These methods are combined with bioinformatics approaches to study the structure and function of macromolecular assemblies involved in a variety of disease processes. Specific research interests are focused on signal transduction processes (Steve Gamblin, Katrin Rittinger, Steve Smerdon), transcriptional regulation (Gamblin, Smerdon, Ian Taylor), DNA damage signalling (Smerdon), innate immunity (Rittinger), influenza (Gamblin) and viral assembly (Taylor).

The cancer research UK biomolecular structure group at The School of Pharmacy (Stephen Neidle, Gary Parkinson), employs crystallography combined with molecular modelling/simulation to study nucleic acids and their interactions with small molecules in the context of anticancer drug discovery. One principal focus is on determination of quadruplex DNA structures, using the derived information to assist in the design of novel telomere-targeting and gene-targeting molecules. Other active structural projects consider protein-protein interactions and anti-infective agents, especially against MRSA.

The crystallographers within the School of Biological and Chemical Sciences at Queen Mary have a focus on photosynthetic reaction centres, plant proteins, enzymes, and proteins produced by bacterial phytopathogens (Richard Pickersgill, Norbert Krauss). The technologies of EPR/ENDOR spectroscopy (Steve Rigby, Peter Heathcote), NMR spectroscopy (John Viles), and electron microscopy (Jon Neild) are combined with crystallography (Pickersgill, Krauss) to understand protein activity and to study systems of greater size and complexity.

At University College, Dept. of Biochemistry and Molecular Biology (which is closely linked to the Birkbeck/UCL Institute of Structural Molecular Biology), X-ray crystallographic studies of biologically important proteins are carried out in conjunction with biophysical characterisation, NMR spectroscopy and bioinformatics investigations. Areas of research include pathogenesis (Gabriel Waksman and Snezana Djordjevic), signal transduction (Waksman and Djordjevic) and enzymatic mechanisms of pathogenic peroxidases (Djordjevic). In addition, neutron and X-ray scattering are used together with analytical ultracentrifugation to determine medium resolution solution structures for immunologically important multidomain proteins (Steve Perkins).

Chemical and materials research

The Industrial Materials group at Birkbeck (Paul Barnes, Nora Leeuw) focus on structure and dynamics of functional materials, with a particular interest in variations of structure on the timescales of about 1 second upwards. Principal techniques include PXRD, especially time-resolved *in situ* methods to study the consequences of chemical or physical changes, energy-dispersive diffraction, neutron diffraction, EXAFS and computer modelling.

Chemical crystallography at UCL (Derek Tocher, Jeremy Cockcroft) underpins research in inorganic and materials chemistry, as well as providing key data for the development of synthetic methods in organic chemistry. UCL is also the principal centre for the Control and Prediction of the Organic Solid State (CPOSS) project led by Sally Price, which aims to develop computational technology for the prediction of the crystal structures of organic molecules.

Research at the Davy Faraday Research Laboratory of the Royal Institution (Richard Catlow, Peter Day, Sir John Meurig Thomas, Paul McMillan, Richard Oldman, Gopinathan Sankar) focuses on solid-state and materials chemistry, including heterogeneous catalysis, surface chemistry, mineralogy, molecular solids and electronic and magnetic materials. The work of the laboratory is based on a combination of experimental and computational techniques, and the laboratory is a major user and developer of national and international central facilities for high performance computing, synchrotron radiation and neutron scattering.

Crystallography in Southeast Universities

At the University of Southampton, chemical crystallography research (Mike Hursthouse, Simon Coles, Thomas Gelbrich, Mark Light) focuses on structural systematics of families of functionalised organic compounds in order to gain insights into crystal assembly, to develop understanding of phenomena such as polymorphism and structural similarity, and to inform work on crystal structure prediction. Typical analyses consider matrices of related structures (often of the order of 100) by systematic approaches embodied in the group's XPac software package, which has been developed to provide an automated gauge of crystal structure similarity. The work is supported by a laboratory developed specifically to examine physical and thermal properties of crystalline solids in order to investigate structure-property relationships and structural transformations. The group is active in the areas of e-science and informatics, developing new approaches to open access publication of crystallographic data (and other analytical data), as well as remote experiment control and systems for data management and experiment analysis.

In Southampton's biological group, Jon Cooper pursues structural studies of various proteins, including enzymes of the tetrapyrrole biosynthesis pathway, C-C bond hydrolases, acute phase proteins, aspartic proteinases, methylotroph electron transport proteins and inositol monophosphatase. Recent projects include structural analysis of a calcium-signalling protein associated with learning and memory, and an invasion protein from the pathogen *Burkholderia pseudomallei*.

At the University of Reading, the research interests of Mike Drew span a broad range of structural chemistry, including small inorganic and organic molecules, metal complexes, host-guest interactions and chiral ruthenium complexes. The main research interest of Christine Cardin has developed into nucleic acid crystallography, focussing in particular on understanding the mode of action of the DACA family of anticancer drugs, developed by Bill Denny at the University of Auckland. The research of Ann Chippindale and Simon Hibble concentrates on ordered crystalline materials such as open-framework metal phosphates, sulphides and cyanides, and disordered crystalline materials, particularly simple transition-metal cyanides. Thermal studies, particularly of negative thermal-expansion materials, and single-crystal-to-single-crystal transformations are a principal research theme.

The functional materials group at the University of Kent (Alan Chadwick, Bob Newport, Gavin Mountjoy) concentrates primarily on atomic-scale structural properties of amorphous and nano-crystalline materials, including bioactive and other oxide glasses, Li-based solid-state battery materials and oxide nano-composites. Inelastic neutron scattering and X-ray absorption spectroscopy complement neutron and X-ray diffraction techniques, with *in situ* and time-resolved experiments becoming a prominent research area.

At the University of Sussex, Darren Thompson is engaged in crystallographic study of proteins in the complement cascade including the multi-protein complex C1, and short switch peptides that have been designed to change conformation from a coil to a finger upon addition of zinc.

At the University of Portsmouth, the main research focus of John McGeehan is on the structural characterization of nucleic acid proteins by macromolecular crystallography in collaboration with Geoff Kneale. He is also involved in collaborative projects with the ESRF and The Diamond Light Source to develop online microspectrophotometers, allowing UV/Vis, fluorescence and Raman spectra to be collected during synchrotron-based macromolecular crystallographic experiments.

Andrew Bond

To be continued in Volume 17, Number 3

AWARDS AND PRIZES

CrSJ 2008 Awards



New honorary members of CrSJ: (left to right) N. Yasouka, F. Iwasaki and M. Tanaka.



Award winners: (left to right) M. Fujihashi, M. Yashima, A. Takenaka (President), and J. Kondo. The General Assembly of the Crystallographic Society of Japan was held in Osaka, Japan during IUCr2008. At the Awards Ceremony, the Prize for Science in Crystallography went to M. Yashima (Tokyo Inst. of Technology) and the Young Crystallographer Awards went to M. Fujihashi (Kyoto U.) and J. Kondo (U. Louis Pasteur). At the general meeting, N. Yasouka (Himeji Inst. of Technology), F. Iwasaki (U. of Electro-Communications), and M. Tanaka (Tohoku U.) became Honorary Members of our society.