

Crystallography News

British Crystallographic Association



Issue No. 124 March 2013

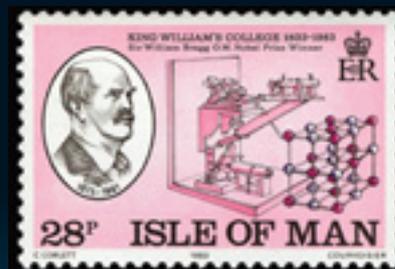
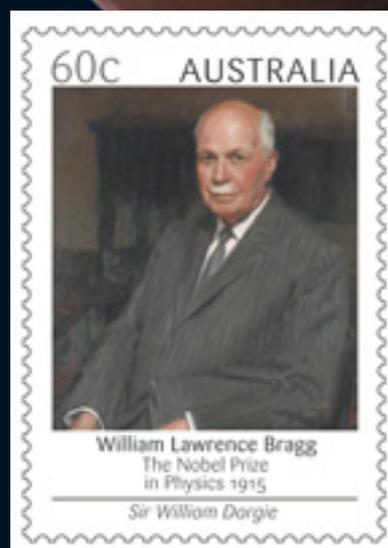
ISSN 1467-2790



X-raying Mars



Honouring the
Braggs



ECM28 Takes Shape

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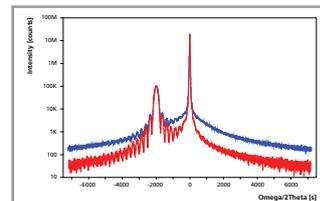
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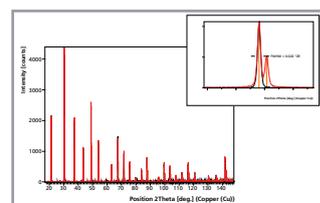
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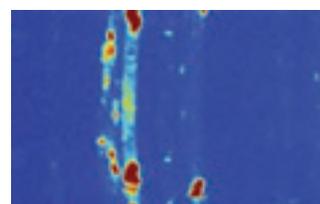
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1D



2D



3D

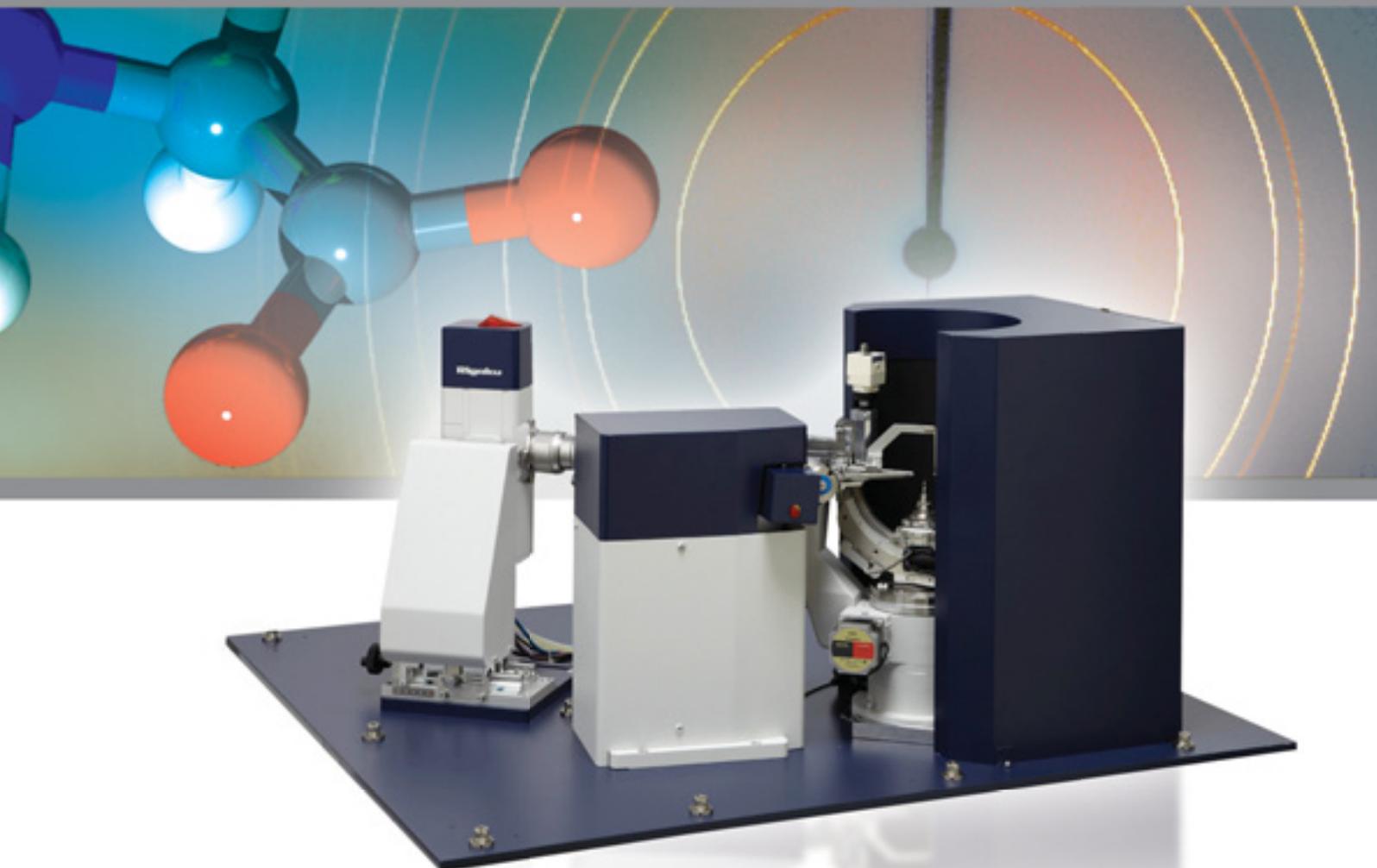


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- A copy of Crystallography News every quarter
- Optional E-mail notifications of news items and meeting information
- Influence on the development of crystallography and the BCA

For current rates, and to join, please see www.crystallography.org.uk/membership/

CRYSTALLOGRAPHY NEWS is published quarterly (March, June, September and December) by the British Crystallographic Association, and printed by Bowmans, Leeds. Text should preferably be sent electronically as MSword documents (any version - .doc, .rtf or .txt files) or else on a PC disk. Diagrams and figures are most welcome, but please send them separately from text as .jpg, .gif, .tif, or .bmp files. Items may include technical articles, news about people (eg awards, honours, retirements etc), reports on past meetings of interest to crystallographers, notices of future meetings, historical reminiscences, letters to the editor, book, hardware or software reviews. Please ensure that items for inclusion in the June 2013 issue are sent to the Editor to arrive before 25 April 2013.

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As required by the DATA PROTECTION ACT, the BCA is notifying members that we store your contact information on a computer database to simplify our administration. These details are not divulged to any others without your permission. You may inspect your entry during the Annual Meeting, or otherwise by application to the BCA Administrative Office. We will be happy to amend entries at any time.

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This month's cover:

Our cover shows the first X-ray diffraction pattern obtained from Mars



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From the President



SITTING in a coffee shop in Cambridge with my daughter just before Christmas I noticed that the festive decorations hanging from the ceiling looked to be snowflakes made out of coins. The problem was that they had five-fold symmetry and just didn't look right. I concluded that they were probably meant to be stars,

but it made me think about how some aspects of crystallography are universally recognised: we expect snowflakes to show hexagonal shapes; gemstones are admired in jewellery; demerara sugar and rock salt crystals are used in the kitchen.

It is the gap between this commonplace crystallography and the work that we "professional" crystallographers do that is sometimes difficult to bridge. However, the gap needn't actually be so large. We can use the Bragg centenary this year to explain how our subject has developed over the past 100 years, through scientific achievements that have reached the general consciousness, such as DNA, penicillin or carbon nanostructures. And next year, with the International Year of Crystallography, we can show the worldwide strength and importance of the subject. With our strong heritage and current relevance we have a good story to tell.

I am therefore delighted at the way people are already taking on the opportunities afforded by the Bragg centenary. Many of us will have already heard **Mike Glazer**, **Chris Hammond** and **Judith Howard** discussing Crystallography with **Melvyn Bragg** (no relation) in the 'In Our Time' programme on Radio 4 last November. If you didn't you can still listen via www.bbc.co.uk/programmes/b01p0s9s. I would like to thank Mike for initiating this excellent programme and for all three of them for being willing to take part. There have also been a number of Bragg-related lectures and day meetings and more are planned, see crystallography.org.uk/bragg-centenary for a calendar of events. The Bragg centenary meeting of the Cambridge Philosophical Society held this January was particularly pertinent given that an earlier meeting of this society was the platform for the first announcement of Bragg's Law. It is also good to see that *Acta Crystallographica A* has just published a series of papers from the Bragg Centennial Symposium held in Adelaide (Lawrence Bragg's birthplace) in December 2012 (*Acta A* **69** (2013) part 1). This is well worth a read, especially the article by Lawrence's daughter **Patience Thomson**.

STFC are also about to publish a short brochure about crystallography to be made available to anyone with an interest in promoting the subject. It is hoped to be ready in time for the Big Bang Fair (ExCeL, London, 14-17 March) where STFC are sponsoring a stand dedicated to crystallography. We are co-ordinating the content through **Ross Harrington** and populating it with enthusiastic demonstrators from our membership and elsewhere. With

around 75,000 young people, teachers and parents passing through the doors over four days it promises to be an exciting – and exhausting – event! Particular thanks are due to Ross for his hard work with this and also to those who have volunteered to help. At the time of writing, places for school parties are fully booked but there are still some tickets available at the weekend for those who can persuade someone from the target audience age-range to accompany them...

Under **Sandy Blake**'s leadership, preparations for ECM28 are gathering pace. It is now possible to register for the meeting, being held in Warwick in August, and up to date information such as the recent announcement of keynote speakers is regularly put on the ECM website (ecm28.ecanews.org/). Similarly accelerating preparations for the Bragg Exhibition – held in Warwick to coincide with ECM28 – are also underway, coordinated by **Mike Glazer** and **Pam Thomas**. This promises to be a fascinating insight into the history of our subject over the past 100 years and should further entice all of us to come to Warwick at the end of August. I look forward to meeting a strong cohort of BCA members at this year's European Crystallographic Meeting on our home soil.

You will no doubt have seen my recent email explaining changes to the BCA Secretary position, with **Georgina Rosair** taking more of a back seat advisory role and **Claire Wilson** becoming acting BCA Secretary. Georgina has an increasing workload as ECA Secretary as the ECM28 meeting approaches and as a result Claire, who was already helping Georgina, is doing more of the BCA Secretary's work. This subtle rearrangement therefore better reflects their current duties and I am extremely grateful to Georgina and Claire for their past and present work in this demanding position.

Finally I would like to highlight some recent work that demonstrates how crystallography has moved from its UK roots and beyond its current global reach. At the end of October last year NASA's Mars rover Curiosity beamed back an x-ray diffraction pattern from Martian soil* (see www.nasa.gov/mission_pages/msl/news/msl20121030.html – pictured on our cover). One hundred years on and we now have an x-ray diffractometer measuring samples on another planet!

I hope that you enjoy reading this issue of Crystallography News.

David Keen

*Ed: an article about how NASA did it appears in this issue.

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(The dates in parentheses indicate the end of the term of office).

Full committee details on the BCA website www.crystallography.org.uk

From the Editor



IN an ordinary year the March issue of *Crystallography News* is the easiest one to fill. About a quarter of the pages are taken up by the final big announcement of the Spring Meeting. During my time as Editor we have been blessed with an unbroken succession of highly efficient Spring Meeting chairpersons. They supplied me with

beautifully balanced spreadsheets, carefully formatted to fill two adjacent pages, flanked by enticing details of the scientific sessions. All I had to do was to give them a quick once-over and send them off to the printers. Of course, this year will be different. Our “Spring Meeting” will take place in August from the 25th to the 29th, and we’ll be joined by lots of our European cousins. We shall find out if any of the trees that beautified the Warwick University campus with their cascades of blossoms in April will bear fruit in August. Registration for this European Crystallographic Meeting is open, and details about it and its satellite meetings can be found at www.ecm28.org.

The European Crystallographic Association is not the only major group that is visiting our shores this year. The even more peripatetic ICCOSS (International Conference on the Chemistry of the Organic Solid State) will be coming to Oxford early in August after meetings in Bangalore two years ago and Sestri Levante on the Genoa Riviera four years ago. After an evening reception at St. Catherine’s College on the 4th of August, the main sessions will take place there from 5th–9th August. The conference will cover research in all aspects of the chemistry and physics of organic solids, including both fundamental properties and applications. Information is available via the website <http://icco2013.org/>. The deadline for Early Bird registration is 31 May.

This year’s meeting of the American Crystallographic Association will take place in Honolulu from July 20 to 24. I intend to submit an abstract and to cover the proceedings for *Crystallography News* (it’s a tough job, but somebody has to do it). The deadline for both submission of abstracts and application for a travel grant is March 31. Early registration ends on May 31.

While all sorts of crystallographers come out to play in the summer, our hardy biological crystallographers make a big splash in the winter. We have a comprehensive meeting report from the CCP4 Study Weekend in January. Once again it bears witness to the ever-increasing power of biological crystallography. There will be further activity in the summer: the South West Structural Biology Consortium will meet at the University of Bristol on July 1–2. More information can be found at <http://www.bris.ac.uk/fmvs/research/swsbc-2013/>.

Since its inception *Acta Crystallographica* has been the gold standard for the publication of crystallographic results. In its

early days quality was guaranteed by the diligence and knowledge of referees from the crystallographic community. Innovatively applying information technology, the IUCr developed CheckCIF to help authors to implement best practice even before referees get involved. As the shift from subscriber-access to open-access journals developed, the IUCr was ready with *Acta Crystallographica, Section E*. Nevertheless, the IUCr journals face another increasing problem. Nowadays much of the most exciting research incorporating crystallographic results is multidisciplinary. Because co-authors who are not crystallographers often prefer non-crystallographic journals, and because crystallographers tend to be amenable rather than argumentative, some results that would be highly appropriate for *Acta Crystallographica* are published elsewhere. To address this problem, the new Editor-in-Chief, **Samar Hasnain**, has developed a plan, which is presented in this issue. Special issues of *Acta Crystallographica, Section A* (about the Braggs) and *Section C* (about absolute structure) are described in additional articles.

This issue contains several articles related to crystallographic history. The most spectacular is the account by our incredibly brave trio of **Mike Glazer, Chris Hammond** and **Judith Howard**, who represented our science to a national audience for the “In Our Time” broadcast on BBC Radio 4 about the Braggs. All of us aspire to give a talk under the benign auspices of the BCA to a courteous and knowledgeable audience of our fellow crystallographers. Many of us are or have been university teachers – a somewhat greater challenge since the audience, even if it has shared objectives and similar background, may sometimes be recalcitrant. Now imagine the challenge of talking with minimal notes to a very large and very diverse unseen audience that could melt away at any moment to make a cup of tea. Our trio, who managed this task triumphantly, describe what it felt like.

We also carry a report on the one-day meeting of the Cambridge Philosophical Society entitled “Bragg’s Law”. Beginning with the Braggs’ earliest discoveries, presentations described both the progress of their scientific careers and some parts of crystallography that came to fruition from the seeds that they planted.

Our December issue featured an article written by **Dennis Beard** with the aid of **Derry Jones** about the experiences of a physics graduate from London who late in the 1940s moved north to a chemistry department in Leeds. One of his most important jobs to which he was appointed by **E Gordon Cox** involved co-ordinating the project team that created a new and more versatile design of Weissenberg camera. I am pleased that this report, and particularly the photograph of a camera that had been acquired by the University of Dundee, prompted **John Low** to write an article for this issue. John describes research in Dundee starting in the late 1960s, for which their two Leeds Cox Weissenberg cameras still were important pieces of apparatus.

Carl Schwalbe



BCA Corporate Membership

The BCA values its close ties with commercial companies involved with crystallography. To enhance these contacts, the BCA offers Corporate Membership. Corporate Membership is available on an annual basis and includes the following benefits:

- Up to 10 free BCA memberships for your employees.
- Ten complimentary copies of the quarterly BCA Newsletter.
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The cost of this membership for 2013 only is **£300.00**.

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Puzzle Corner

THE necessary clues can be found in this issue, relevant websites or general crystallographic knowledge. Find the values of W, X, Y and Z, and hence derive the final answer.

1. Start with the seating capacity of the main lecture theatre at Warwick Arts Centre, the venue for ECM28.
2. Divide this number by the date in August on which ECM28 starts to get number W.
3. Multiply W by the cost in pounds to register for the European Young Crystallographers Meeting, yielding X.
4. Multiply the date in May that is the last chance for Early Bird registration by the highest number for a microsposium at ECM27 (in Bergen). Add X to this product to obtain Y.
5. Subtract the number of Sohncke space groups from Y. Then add the number of Bravais lattices, producing Z.
6. Take the first three digits of the ISBN for the book "Drive and Curiosity..." Subtract Z from it. Take the positive square root to get the number of Braggs featured on the "In Our Time" programme broadcast of November 29.

ANSWER to the December 2012 Seasonal Codeword
There are joint winners: **Derry Jones** and **Jim Trotter**.

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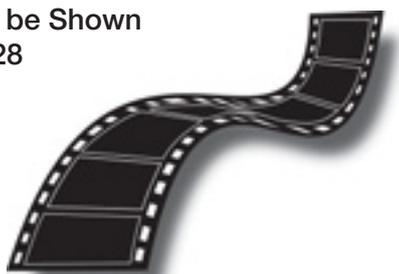
Information about this year's European Crystallographic Meeting



25 – 29 August 2013

THE Organising Committee are hard at work producing a really exciting programme. Please consult www.ecm28.org regularly for updates. Registration is now open, and participants should note that 6 May is the cut-off date for Early Bird registration.

Films to be Shown at ECM28



“Driven to Diffraction”

~55 minutes

THE documentary film *Driven to Diffraction* tells the remarkable story of **William Henry Bragg** and his son **William Lawrence Bragg**. Part human interest story, part science lesson, part historical journey of discovery, the film weaves a spell of enchantment around the tale of two shy men who join the ranks of the most important scientists of the twentieth century.

From origins in Adelaide, their international contributions have been legion and across many areas: early work on wireless telegraphy, radioactivity, and acoustic range finding of artillery on the battlefields of the Great War, to their celebrated development of X-Ray crystallography, for which they won the Nobel Prize in 1915, the only father-son team ever to have done so.

Their work made possible an astonishing list of breakthroughs including Watson and Crick's discovery of the structure of DNA, radio therapy for cancer, solid state electronics, modern pharmaceuticals, superconductivity and radio astronomy.

“Naturally Obsessed – the making of a scientist” ~60 minutes

THIS follows a small group of protein crystallography PhD students at Columbia over the course of months/years.

Mixing humour and heartbreak, *Naturally Obsessed: The Making of a Scientist* delves into the lab of charismatic professor **Dr Lawrence Shapiro**, and follows three irrepressible graduate students on their determined pursuit of a PhD and scientific success.

“Il misterio de los cristales gigantes” (the mystery of the giant crystals)

~ 50 minutes

NARRATED in Spanish, Italian, French, English.

Some of these crystalline structures of quartz are more than 10m long and 1m wide.

Careers Session at ECM28

THE “careers session” will run for an hour and will involve four 10 minute talks from “early career” European crystallographers and structural scientists who have recently obtained permanent posts in either industry or academia within Europe. We have selected speakers with four different career paths to give the target audience of post-doctoral and graduate students a flavour of the career options that are open to them. The remaining 20 minutes will be run as a discussion session with the four speakers acting as a panel to answer questions from the audience.



THE IUCr has initiated a major project to extend and expand the scope of its Journals to meet the needs and serve the interests of the crystallographic and wider scientific community that utilize structural information for addressing their scientific questions. The Editor-in-chief, Samar Hasnain, appointed in August 2012, in consultation with appropriate committees and commissions of the IUCr as well as the wider structural science community has developed a plan to make the IUCr's journals the natural home for many of the high-quality scientific publications that are currently published in NSMB, Structure, PNAS, JACS, Angewandte Chem., Chem. Commun., etc, where structural data underpin these publications. The overall plan was recommended by the Finance committee in October 2012 and approved by the Executive Committee in December 2012.

Chemists, biologists, physicists and material scientists will be actively encouraged to report the best of their structural studies in the IUCr's journals. Significant changes are being implemented in Journal organization and management to coincide with the celebration of the International Year of Crystallography. Major scientific advances require multidisciplinary research and very often these breakthrough papers report results covering a wide range of methods and technologies. The wide ranging expertise that exists on our editorial boards is being further strengthened by bringing additional research leaders in Chemistry, Crystal Engineering, Biological Sciences, Materials Science, Free Electron Laser Science and Technology and broader range of structural methods so that our journals continue to lead on all aspects of structural science and methods. *Acta Crystallographica* journals subtitles are being made more explicit to reflect the fact that we are open to publishing wider range of science than the perception by the wider scientific communities. The first issue of *Acta Crystallographica B* under its new sub-title *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials* appeared on 1 February 2013. ACTA A, C, F and possibly D are expected to follow soon.

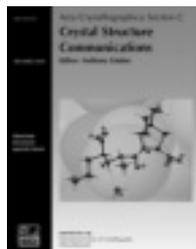
Because crystallographic studies are critical to understanding the structural basis for chemistry, physics, biology, and materials science the IUCr will inaugurate a new journal as part of the celebration of the IYCr. The new Journal will be simply called "IUCr Journal" (IUCrJ). IUCrJ will be fully open access striving to reach high impact and influence appropriate for the best of our structural sciences. Our aim is to capture a fair share of high profile papers on all aspects of sciences, technologies and methods supported by IUCr via its commissions including emerging fields such as 3D structures from 'single molecule' by the next generation of Free Electron Lasers. Much of the exciting structural science results that are published in other high profile journals appeared first in presentations at IUCr congresses, AsCA, ECM, and ACA meetings. The goal for 2014 will be to publish 100 articles in IUCrJ covering as many aspects of structural methods development and application as possible. IUCrJ should become the natural home for reporting breakthroughs and 'full' science reports rather than simply the structure or how it was determined. As much as half of these will be solicited from the presentations of cutting edge research at ACA, ECM, AsCA meetings as well as the IUCr congress and conferences closely linked to IUCr via their commissions such as BSR, SAS etc.

A Management Board has been appointed including the main editors of the current Journals, IUCr's President, Treasurer & Secretary General and **Professor Mitchell Guss** as an additional representative of the EC. The board is responsible for (a) increasing the influence of IUCr journals among the wider scientific communities (b) serving the interests of all of its Commissions, (c) broadening the scope of the journals so that high quality science papers that use crystallography are attracted to the journals, and (d) improving the visibility of IUCr journals at non-crystallographic conferences.

A Business Development Manager will be appointed in early 2013 with a mandate to (a) reach out to wider science community, (b) encourage closer integration of the journals with the Commissions, (c) develop social media marketing, (d) boost article citations by writing press releases highlighting the most significant papers, (e) prepare market research reports including citation and usage trend analysis, (f) identify subject trends and new journal opportunities, (g) identify target authors and encourage them to submit to the journals, and (h) exploit opportunities arising from IYCr2014. The Business Development Manager will work closely with the Editorial staff.

Samar Hasnain
Editor-in-Chief

Acta C: Virtual issue on absolute structure



Following the success of the inaugural virtual issue on polymorphism in December 2011 (http://journals.iucr.org/special_issues/2011/polymorphism/), *Acta Crystallographica Section C* is pleased to release its second virtual issue, which is on the topic of absolute structure (http://journals.iucr.org/special_issues/2012/absolutestructure/). The unambiguous determination of absolute structure, particularly where the absolute configuration of an enantiomerically pure chiral molecule is needed, is important not only for synthetic and natural-product chemists, who wish to fully characterize their products, but can be a critical step for the pharmaceutical industry, where opposite enantiomers of a drug can have quite different biological properties. One should also mention those crystal engineers endeavouring to prepare non-centrosymmetric crystals for applications such as second-harmonic generation.

A major impetus in enabling the study of absolute structure has been the advent of dual radiation CCD diffractometers. This means that more laboratories have routine access to Cu K α radiation with the potential to successfully study light-atom structures. The latter have been viewed as one of the remaining difficulties in this field.

Acta A: Open-access articles commemorating the Bragg centennial

The first 11 articles in the January issue (Volume 69, Part 1) of this journal form a collection of articles contributed by speakers at the Bragg Centennial Symposium held in Adelaide on 6 December 2012. This symposium aimed to explore some of the historical context and personal links to the Braggs' work, as well as its broader scientific and social impact. In the words of the first author, **S W Wilkins**, "11 November 2012 marks the centenary of the reading of the paper by William Lawrence Bragg (WLB) to the Cambridge Philosophical Society outlining the foundations of X-ray crystallography. It included the derivation of the first correct atomic structure of a crystal, namely that of zinc blende, based on the X-ray diffraction pattern recorded by **Friedrich, Knipping** and **Laue** in the spring of 1912. At the time of the lecture, **Lawrence Bragg** (as he later preferred to be called) was 22 years old and still a research student in the Cavendish Laboratory.

For the validation of absolute-structure determination, over the years there has been a heavy reliance on the statistics (values and standard uncertainties) of derived parameters or something equivalent, and little study of the fit of the model to the observed quantities. There has been little questioning of the quality of crystals, data collection and correction methodologies. Clearly, absolute-structure determination is still a rich field, wide open for development, especially for light-atom compounds of great importance to the pharmaceutical and chemical industries.

The concept of virtual issues of *Section C* is an initiative designed to make it easier for readers to find papers relevant to their field of interest, thus increasing the visibility and impact of those papers, and consequently the attractiveness of the journal to authors. This virtual issue has the ambition to present the results of crystal-structure determinations which demonstrate new successes and remaining limitations in absolute-structure evaluation.

The editors of *Acta Crystallographica Section C* hope that readers find this virtual issue interesting and beneficial. The next virtual issue, on the subject of metal-organic frameworks, will be published in late 2013.

Anthony Linden
Editor of *Acta Crystallographica Section C*
University of Zurich, Switzerland

Howard D Flack
Guest Editor of the virtual issue on absolute structure
University of Geneva, Switzerland



This special issue of *Acta Crystallographica Section A* is dedicated to commemorating this landmark scientific event, the ramifications of which have served as a wellspring for many other branches of science, including structural chemistry, mineralogy, materials science, solid-state physics and molecular biology. It is very fitting that a Bragg centennial issue be published in *Acta Crystallographica*, as it was Lawrence Bragg who was a major influence behind the formation of the International Union of Crystallography (IUCr) and *Acta Crystallographica* more than six decades ago. Lawrence Bragg also served as the inaugural President of the IUCr Executive Committee. A sense of the development of crystallography over the past six decades can be obtained by looking at the most frequently cited articles in *Acta Crystallographica* as listed on the IUCr Journals website."



X-raying Mars: How NASA Did It

WE crystallographers know that X-ray powder diffraction is the method of choice for identifying polycrystalline samples. However, those of us who grew up with previous generations of diffractometers expected them to be housed in a cubicle the size of a small room and to require the regular attention of a friendly service engineer. Plainly this technique would be immensely valuable for identifying rock samples on the surface of Mars, but such an application seemed to belong to science fiction. Therefore, when Rob Delhez from Delft gave a Plenary Lecture at the 2008 BCA Spring Meeting with the title “X-ray Diffraction on Mars?”, there was a packed audience. Rob told us about the instruments developed for Mars exploration by NASA and ESA and thrilled us with his description of the technological breakthroughs being achieved. Even so, we wondered if any instrument light enough for interplanetary transport could be robust enough to withstand the physical and thermal shocks it would encounter. The diffraction pattern from a Martian sample on our cover proves that the CheMin (Chemistry & Mineralogy) instrument on the Curiosity rover did just that.

Starting with a prototype to prove the principle, CheMin went through a series of iterations to reduce size and weight while increasing versatility. The first version used a commercial X-ray tube tower and a commercial CCD camera in an evacuated housing, and it had separate bulky electronics and power supply. The second version saved space by interfacing the X-ray tube and power supply to the camera with the sample kept under ambient conditions and the X-rays entering the camera through a beryllium window. As with conventional powder diffraction, the required state of the sample was very demanding: the particle size had to be as fine as flour, 10 μm or less. Allocating space, mass and electrical power for the requisite grinding equipment would take up resources that could be more productively utilised by other scientific apparatus. A breakthrough with the third-generation CheMin solved this problem. Simple sieving of material brought up by scooping or drilling can limit the maximum particle size to 150 μm . This still relatively coarse sample was spread between two parallel Mylar or Kapton films about 200 μm apart held between the prongs of a “tuning fork” with a piezo-electric actuator. The vibration made the particles tumble enough to ensure random orientation. Integration and miniaturisation made big advances in the fourth generation, which featured an integrated microcomputer, on-board lithium-ion batteries and a power management system. CheMin IV was successfully field-tested in 2006 on an expedition to Svalbard, Norway, at nearly 80° north latitude. Not only did it withstand the low temperatures there, but also it demonstrated the unique advantage of *in situ* autonomous operation for terrestrial as well as interplanetary geochemistry. If data from a sample appeared to be ambiguous or exceptionally interesting, another sample could be taken nearby and retested.

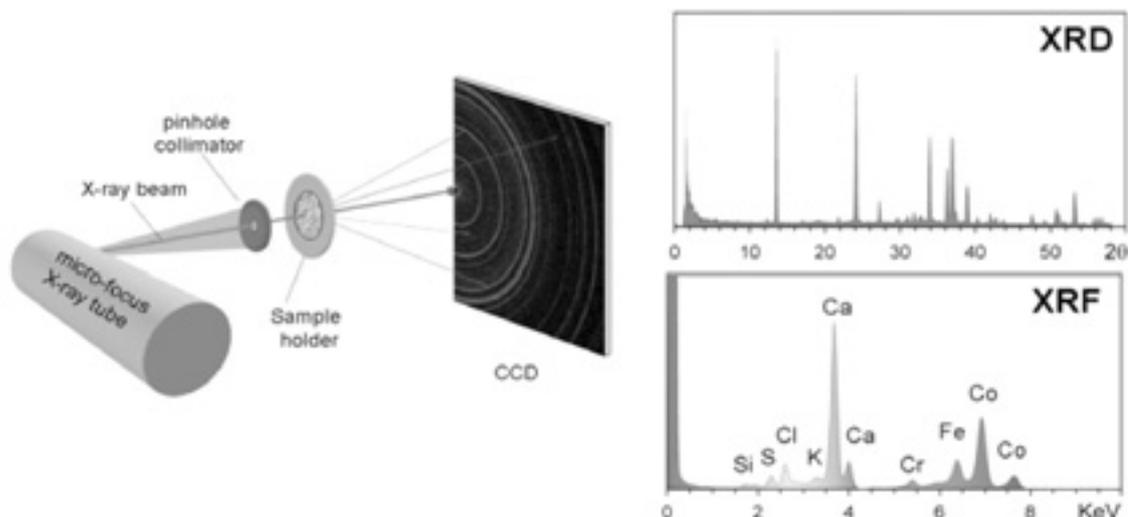
Normally such results would only become known after the samples had been returned to the parent laboratory, necessitating a return visit on another expedition.

The flight model (FM) of CheMin was built at the Jet Propulsion Laboratory between 2005 and 2009 and delivered in June, 2010. Its design specification required it to operate for one Martian year; spares of critical components were tested to survive 1.5 times this time span. As well as the external hazards, the Curiosity rover inflicted an additional hazard on the components of its Mars Science Laboratory (MSL). The Radioisotope Thermoelectric Generator that provides the instruments with a steady supply of power, unaffected by day-night cycles or dust storms, also irradiates them with an unwanted flux of neutrons. Our cover picture of the installation of CheMin into Curiosity demonstrates two things: the great care taken to avoid contamination or damage, and the remarkable degree of miniaturisation. The shape and size of FM approximate to a cube 25 cm on a side, and its mass is about 10 kg. An identical twin of FM called the demonstration model (DM) has been built for use in testing analogues of Martian samples as well as duplicating and analysing possible “glitches” in the operation of the instrument. Samples of known composition thought likely to resemble those to be found on Mars were analysed with the DM, and the resulting data were used for calibration. Curiosity was launched on 26 November 2011 and landed on Mars on 5 August 2012.

The source of X-rays for CheMin is a microfocus Co X-ray tube operating at 28 kV which produces a beam approximately 50 μm in diameter through a pinhole collimator (Fig. 1). The CCD detector has pixels 40 x 40 μm^2 . It is placed on the opposite side of the sample from the source and is read out at such a high frequency that pixels almost always contain charge from zero or one photon. The two-dimensional diffraction pattern can be summed circumferentially around the direct beam position to yield a conventional XRD plot of intensity versus 2θ . Measurement in the forward-scattering mode captures the most intense diffraction peaks and enables minerals with large interplanar spacings and hence low 2θ values such as layer silicates to be detected. Although a capability to do elemental analysis by X-ray fluorescence (XRF) was part of the original project specification, it was subsequently deleted. Nevertheless, the ability to measure energy per photon makes it possible to plot energy-dispersive X-ray histograms.

According to the specifications, the XRD function of CheMin should be able to detect individual minerals comprising 3% or more of a sample. For minerals present at 12% or more, the accuracy should be $\pm 15\%$ of the analytical value; and the precision, $\pm 10\%$. Due to the transmission geometry and the use of Mylar or Kapton windows, the XRF function is only capable of detecting elements with atomic number > 12 (starting with Al).

Figure 1. Schematic diagram of the CheMin geometry and the XRD and XRF traces it can produce (courtesy of NASA/JPL-Caltech/Ames).



In operation, a sample is sieved and about 10 mm³ is delivered to one of the 13 cells with Kapton windows (more durable) or 14 cells with Mylar windows (less X-ray background). An additional five cells contain calibration standards. X-ray measurements are made at night when the CCD can be cooled to -60°C to eliminate dark current and reduce damage by stray neutrons. The analysis time for each sample will range from a few to >10 hours. To reduce the load on the communications back to Earth, initial data processing is carried out by the on-board electronics and only data products are transmitted. The sample cells can be reused once or twice more. After a satisfactory analysis has been obtained, the sample is ejected to a sump. To minimise cross-contamination, it is possible to “rinse” the cell with some of the next powdered sample before material is retained for analysis.

Our cover shows the first X-ray diffraction pattern obtained from Mars. The sample came from a patch of dust and sand named Rocknest. The dust is redistributed globally by storms; the sand originated locally but is still thought to be modern. The pattern is coloured by intensity, red signifying

the greatest intensity. It shows significant amounts of feldspar, pyroxene and olivine, while about half the sample is non-crystalline volcanic glass or its weathering products. This composition is similar to that of weathered basaltic soils of volcanic origin found in Hawaii. For those of us who like to imagine ourselves as astronauts this provides an additional incentive to attend this summer's ACA meeting!

Carl Schwalbe

The author has abstracted this account from websites provided by NASA/JPL-Caltech and the Geochemical Society, accessed 2 February 2013:

<http://msl-scicorner.jpl.nasa.gov/Instruments/CheMin/>

http://www.geochemsoc.org/publications/geochemical_news/gn144sep10/ahistoricalperspectiveofth/

The interested reader is encouraged to consult these websites, which provide much further interesting detail.

Images courtesy of NASA/JPL-Caltech.

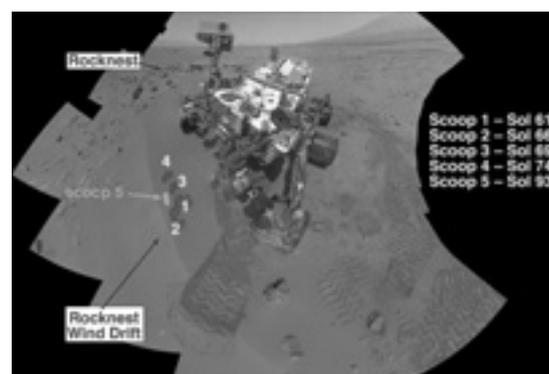
Figure 2. CheMin sample holders



Figure 3. CheMin CCD



Figure 4. Curiosity's “Rocknest” workplace on Mars showing where samples were scooped.



Crystallographic History: Celebrating the Braggs

In Our Time – What the Braggs did for us

WE are now embarking on a period in which we will be celebrating the centenary of the seminal discoveries of **Max von Laue, William Henry Bragg** and his son **William Lawrence Bragg**. As part of this celebration it was decided to approach the producers of the programme “In Our Time”, hosted by the brilliant **Melvyn Bragg** (who was, by the way, born in Wigton, Cumbria, like **William Bragg** too!). This particular programme is one of the few in the media that has a fine record in discussing the arts and sciences at a reasonably high intellectual level. In the event a quick response was received from one of the producers, **Tom Morris**, at the BBC expressing interest in doing something on crystallography and so entered into a series of joint discussions to see what such a programme would entail. It became very clear that, after supplying him with a long list of possible topics, ranging from the early history through to the discovery of X-rays and X-ray diffraction and the work and influence of the Braggs up to the present day, because of the vast range covered under the title of ‘Crystallography’, this was going to be a seriously demanding operation: “In Our Time” lasts just 43 minutes on a Thursday morning and so time is very limited. This meant that we had to be able to select material that would make a coherent story that would not only be informative but also convey the excitement and importance of crystallography. Describing on the radio what is a very visual subject was going to be quite a challenge.

The principal producer for our particular episode, **Natalia Fernandez**, was extremely enthusiastic about this project, but had the immensely difficult and unenviable job of understanding and sorting out all the details. After several very long telephone calls to each of us, she came up with a running order. It was decided that Judith would start by explaining what crystallography is and possibly by discussing some of the early history. This would be followed by Chris talking about the discovery of X-rays and the work of Laue, Friedrich and Knipping in early 1912. Mike was then given the task of explaining who the two Braggs were and what they did.

It should be realised that although there is a running order, it is not strictly adhered to, and Melvyn Bragg is extremely adept at steering the conversation at a slick rate and one has to be prepared to discuss ad hoc ideas as they come up. This requires one to think quickly before responding. There is no rehearsal for this programme. Furthermore we learnt that we could not take notes into the studio with us (at least not on sheets of paper because the microphones were very sensitive and would pick up any rustling of papers, although we could bring in a few notes on a couple of cards). And given that this would be going out live to many millions of listeners, it became a daunting prospect! None of

us have had any experience in broadcasting, and we all three viewed the approaching event with much trepidation. Just what had we got ourselves into? Would any of us clam up at a critical moment, forget names or dates or details, or more seriously make a mistake? And then we had visions that after the programme we would get emails complaining that this or that was wrong.

The programme was due to go out just after 9 am on 29 November and the BBC arranged for Mike and Chris to stay overnight in London. Judith had to come down from Durham, but because of the floods most of her trains were cancelled and so she arrived very late into London. This meant that while Mike and Chris had time over an Indian meal the evening before to chat over the topics to be discussed, Judith was unable to participate in this way in advance of the programme. We had been instructed to turn up at Broadcasting House at 8.30am and we were then taken up to the studio suite. This was rather new and smart and the producers, Natalia, and another of the producers, Victoria, made us very welcome with tea or coffee, cakes and fruit. A few minutes before the programme was due to begin, and after Melvyn had made his customary trailer during the Today Programme, we were led into the studio: a bit like entering an operating theatre! Once inside, we were each given a comfortable chair at a round table with a microphone in front of each of us. Melvyn sat at the head of the table and chatted with us for a few minutes, explaining how he saw the structure of the programme.

At the exact time, Melvyn gave a brief introduction, quoting a passage from **Max Perutz** to set the scene, and then the session started. Judith explained what crystallography is, followed by Chris on X-rays and Laue. Mike then described Lawrence Bragg’s seminal November 11th paper to the Cambridge Philosophical Society, written at the tender age of 22 years. Interestingly, despite our trepidation, we all three very quickly relaxed and forgot that we were on air. Melvyn put us at our ease by treating the whole programme as a conversation between equals. Time flew past very quickly – and suddenly the programme had ended!

At this point Natalia came in very excitedly to tell us that they had been receiving lots of positive tweets while we were talking. In fact almost all the comments we have received were favourable, and in particular they showed that we had managed to put over the message (with relatively few gaffes, we hope) that crystallography is an important, exciting and modern field of science.

We are grateful to Melvyn Bragg and his team at “In Our Time” for making us so welcome at the BBC.

Mike Glazer, Chris Hammond and Judith Howard

The broadcast can be heard at <http://www.bbc.co.uk/programmes/b01p0s9s>.

Bragging about the Braggs

ON 11 November 1912 the great **JJ Thomson** presented a paper to The Cambridge Philosophical Society on behalf of a young fresh graduate, the effect of which can truly be said to have changed the world. The young man, a mere 22 years old, was **William Lawrence Bragg**, and his paper showed for the first time how to interpret the x-ray diffraction experiments of **Laue, Friedrich and Knipping** carried out earlier that year; and furthermore he produced the first example of a crystal structure determination, in this case that of **ZnS**. Thus was born the modern era of crystallography. The paper appeared in print at the beginning of 1913, and was followed by several others, sometimes with his father **William Henry Bragg**, in which the ionization spectrometer (a forerunner of the modern diffractometer) was used, and in which structures such as sodium chloride and diamond were described.

This year on 11 January the Cambridge Philosophical Society held a one-day meeting entitled "Bragg's Law" at the Cavendish Laboratory. As part of my own personal interest in all things Braggian, I decided to attend the meeting. It was an especially nostalgic meeting for me, because I was able to meet up with some of my old Cavendish Laboratory colleagues from 36 years ago; but more importantly the occasion was an opportunity to join in the celebrations. It was a pleasure also to see many members of the Bragg family present.

The meeting was introduced with a short talk by **Haroon Ahmed** from the Cavendish Laboratory who gave a brief history of the 1912 meeting, including a slide of the agenda and meeting notes taken at the time. As far as I know these have never been published. This was followed by **Sir John Meurig Thomas** (Cambridge), who had some years back been a director of the Royal Institution (both WL and WH Bragg had also occupied that post in their time). He gave a fascinating outline of the history of the discovery by both Braggs and the early developments that followed. After this **Judith Howard** (Durham) discussed "What would Bragg have done with neutrons?", an interesting and thought provoking title. Judith showed nicely how neutron diffraction is a natural adjunct to x-ray diffraction but conveys complementary and useful results.

The next speaker was **Sir Peter Hirsch** (Oxford), who gave a humorous and lively description of his time at the Cavendish Laboratory working with Lawrence Bragg, and how electron diffraction developed as a consequence of x-ray diffraction. He had several anecdotes that amused everyone. I hadn't seen him for many years, but I was delighted to see that he is still as sprightly as ever! Following him came **Archie Howie** (Cavendish Laboratory) to talk on channelling of waves and particles and how, through electron diffraction, it is possible to image the crystal planes used by Bragg in his derivation of his famous law.

Richard Henderson (Laboratory of Molecular Biology, Cambridge) talked about structure determination of biological molecules with emphasis on x-ray and cryomicroscopy, thus demonstrating how far that original work of the Braggs has taken us. **John Rodenburg** (Sheffield) then introduced the

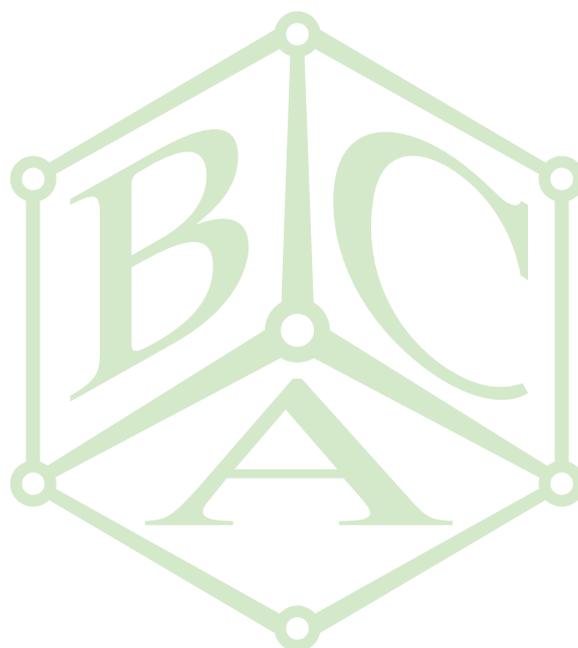
idea of imaging in electron microscopy and phase retrieval without the use of lenses. We all learnt a new word, at least to me: ptychography (look it up on the internet!).

After tea, **John Spence** (Arizona and Lawrence Berkeley), who had flown over especially for the event, gave an astounding description of femtosecond pulsed x-ray crystallography. I loved the title "Diffract and destroy". For the uninitiated this is where one uses a high intensity series of pulses of x-rays that destroy tiny crystals injected across the x-ray beam, such that each crystal gives a distinct diffraction pattern just before it is destroyed. Then with thousands of such patterns, all from different crystal orientations, modern computer power is used to sort this all out and derive the protein structure. The Braggs would have been overcome with excitement to see how their work had led to such an advance. It is a far cry from the way we did x-ray diffraction when I first started!

Finally, **Jeremy Baumberg** (Cambridge) discussed diffraction from photonic crystals, especially those found in nature, for example in butterfly wings etc. Very colourful, interesting and sometimes peculiar!

In short, this was a memorable occasion, which did great honour to the memory of the two Braggs.

Mike Glazer
Oxford & Warwick



Celebrating Weissenberg and His Camera

Addendum to DS Beard and Weissenberg Goniometers

FOLLOWING WEISSENBERG'S 1924 INVENTION OF THE MOVING-FILM CAMERA, SEVERAL INDIVIDUAL CRYSTALLOGRAPHERS IN THE 1940S AND 1950S DESIGNED APPARATUS.

THE equi-inclination moving-film technique of recording X-ray reflexions from separate layer lines was devised by **Karl Weissenberg** (1893-1976) who had been in the group of **Michael Polanyi** (of Schiebold and Polanyi and father of Nobel prizewinner **John Polanyi**) at the Fibre Research Institute in Berlin. Born in Austria, Weissenberg had to leave Germany in the 1930s and, via Paris, came to England. At the BCIRA, Shirley Institute in Didsbury, Manchester, he developed the textile (Weissenberg) rheogoniometer; I suspect that few there knew of his earlier X-ray achievement. **Andrea Sella** has recently published a page on Weissenberg in *Chem World* 8 60 (2011).

WA Wooster and **AJP Martin** (later to win the Nobel Prize for chromatography) described in *Proc Roy Soc A* in 1936 a two-crystal Weissenberg (the experimental and a reference crystal came alternately into the beam as a means of

standardizing intensities); their design was probably the basis of the Unicam Weissenberg that the Leeds instrument was intended to improve on. In 1936 also, **MJ Buerger** published in *Z Krist(A)* 94 information about a massive (with cast-iron bases) equi-inclination Weissenberg, with effective film diameter 5.73 cm, and illustrated it again in his *X-ray Crystallography* (Wiley, 1942). What appears to be a commercial version (Charles Supper & Co) is illustrated in **GH Stout** and **LH Jensen** *X-ray Structure Determination* (Macmillan, 1968) and a price range for Weissenbergs of \$ 1400-3500 is quoted. In the 1940s and 50s, several Weissenberg designs appeared in *J Sci Instrum*, from **RG Wood** and **G Williams** in 1944 onwards. Just before the Cox, Beard and Sutton paper appeared (incidentally, my quotation dated 9 Sept, 1952, from Hilger and Watts for the Leeds Weissenberg was GBP 750), **A McL Mathieson**, at CSIRO Melbourne, described a horizontal (for operation with a GE X-ray set) equi-inclination instrument in April 1951 (though the original draft was submitted 1949). Just after the Leeds paper, **CA Beevers** published in July 1952 a vertical (to suit a Raymax X-ray set) normal-beam (not equi-inclination) Weissenberg, with a larger 10 cm camera diameter, said to have been built at Manchester in 1938 and by Unicam for Edinburgh in 1950-51.

Derry W Jones
University of Bradford

Weissenberg photography and other crystallographic work at Dundee

THE picture in the December issue of the Dundee University Leeds Cox Weissenberg Camera brought back many memories.

I joined Dundee University as a Technical Officer in November 1967, and the Weissenberg camera in the picture was then being used in conjunction with a Wooster 4-circle diffractometer¹ and a Hilger and Watts Linear diffractometer. The camera and the Wooster diffractometer were in the Chemistry Department, and the Linear Diffractometer was shared with the Physics department in which there was also a Leeds Cox Weissenberg camera.

I was appointed to both departments, for which my main function was to run and prepare crystals for the Linear Diffractometer. **John Iball**² was in charge of the Chemistry crystallographic group and **Herbert Wilson**³ was in charge of the Physics group.

John Iball worked with **WH Bragg** at the Royal Institution but had already made a name for himself in the field of polycyclic aromatic compounds and their carcinogenicity. He developed a scale for the measurement of the relative potency of carcinogenic compounds, 'the Iball index', which is defined as the percentage of skin cancer in mice (skin painting experiments) divided by the average latent period in days for the affected animals multiplied by 100.

The main focus of the chemistry group when I joined was on the determination or re-determination of the structures of anthracene derivatives and other planar polycyclic hydrocarbons. Many data sets were collected on the Leeds camera using multiple film packs, and then the intensities were measured by visual estimation or by the use of a scanning microdensitometer. The integration feature on the camera was a real necessity here; however, both procedures were extremely labour intensive. Although the use of the diffractometers reduced the need for visual estimation and the use of film packs, Weissenberg photos were still required for the setting of crystals and determination of lattice parameters prior to putting the crystals on the diffractometers. A nice feature was that there was a small camera which could take oscillation photographs used in setting the

crystals prior to taking Weissenberg photographs or in aligning crystals before putting them on the diffractometers.

Seeing the camera again revived memories of the smell of and time that was spent in the darkroom. This was essentially a broom cupboard fitted under stairs and had room for at most two people. Preparation of film, cutting to size, was all carried out under a very dim green safelight while the film was still in its wrappers; but this light was put out when the film was put into the camera, so this procedure was carried out in pitch darkness using only the sense of touch. This could be tricky especially with a pack of four films. It was obviously of crucial importance to make sure that the film was completely light tight. This was done by feeling round the edge of the cassette into which the film was fitted to make sure that there were no wrinkles in the masking paper. Accidents did happen and every so often films were developed after a 24 hour exposure only to find out that they were completely fogged... this did not make one very popular!

At this time Dundee University or as it was for part of the time described, Queens College, University of St Andrews, had two thriving crystallography research groups. When I

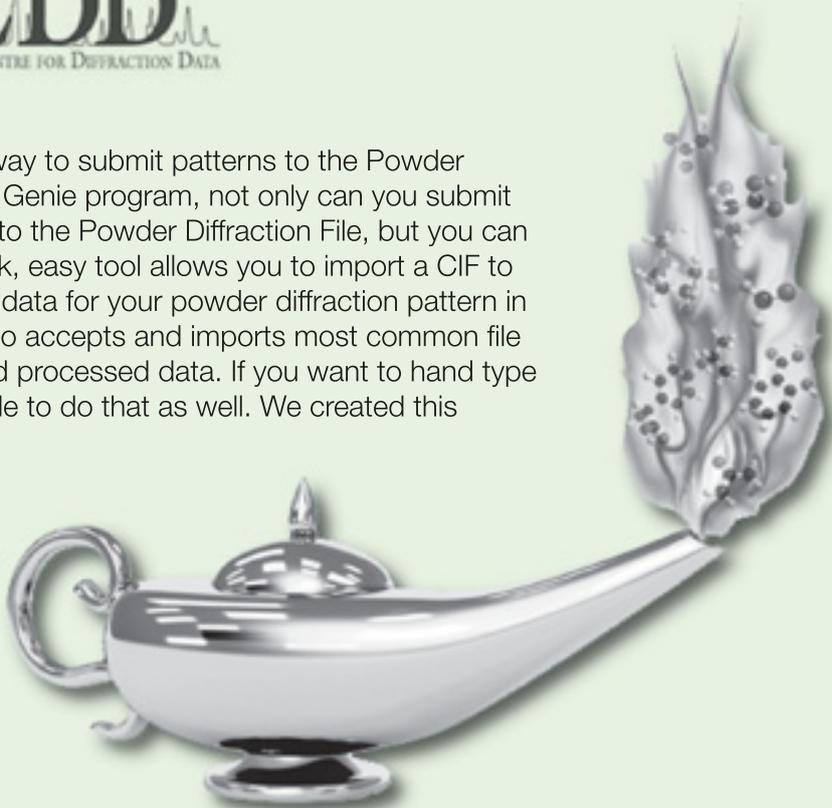
first joined, the chemistry group included **Sam Motherwell**, who was then a post-doc, and slightly later **Sheelagh Scrimgeour**, who was later Organic Section Editor of Structure Reports under the editorship of first **John Iball** and then **George Ferguson** who was a frequent visitor to the Lab. Later **John Barnes** took over when John retired, and he and **Tim Weakley** became very active crystallographers. During all this period the Leeds Cox Weissenberg was in daily use until the availability and cost of film became a problem. When a national diffractometer data collection service at Cardiff became available, the Weissenberg was given pride of place in the Dundee University Museum.

- 1 Crystal Structures Ltd. 1962 J. Sci. Instrum. 39 538
- 2 http://www.royalsoced.org.uk/cms/files/fellows/obits_alpha/iball_john.pdf
- 3 http://en.wikipedia.org/wiki/Herbert_Wilson

John Low



Genie is ICDD's newest way to submit patterns to the Powder Diffraction File™. With the Genie program, not only can you submit your high-quality patterns to the Powder Diffraction File, but you can do so with ease. This quick, easy tool allows you to import a CIF to read in all crystallographic data for your powder diffraction pattern in one step. The program also accepts and imports most common file types for raw data files and processed data. If you want to hand type the information you are able to do that as well. We created this program with you in mind.



As always, we appreciate receiving your feedback and submissions.

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News from the Groups



CCP4 at Nottingham

THE annual Collaborative Computational Project in Macromolecular Crystallography (CCP4) Study Weekend was held at the East Midlands Conference Centre at the University of Nottingham on 3-5 January, 2013. This year's meeting, entitled "Molecular Replacements", provided a comprehensive overview of the technique, including introductory tutorials, emerging methodologies and future challenges. The scientific programme was organised by **Helen Walden** (Cancer Research, UK) and **Pietro Roversi** (University of Oxford, UK) with advisory input from **Airlie McCoy** (University of Cambridge, UK). Registered participants numbered 357 and drew scientists from a diverse range of academic and industrial institutions in the UK and from 15 other European countries as well as Canada, China including Hong Kong, India, and the United States.

The meeting was opened by CCP4 Scientific Coordinator **Keith Wilson** (University of York, UK), with a thoughtful remembrance of three influential macromolecular crystallographers who passed away in 2012: Dame Louise Johnson, Professor Guy Dodson and Professor Roger Fourme. Obituaries for Louise and Guy can be found in the previous and current BCA newsletter. An excellent description of Roger Fourme's career and scientific contributions can be found on the IUCr website (<http://www.iucr.org/index.html/leading-article/2013/2013-02-07>).

The first session opened with a talk by the current chair of CCP4 and Working Group 1, **Martin Noble** (Newcastle University, UK). In his talk entitled "Introduction to MR," he described the molecular replacement (MR) operation as a *Phase Transplant* from a *Phase Donor* (the search model) to the *Phase Recipient* (the unknown structure). This operation is needed when the two models are similar but not near identical, and when access to phases is not available experimentally through SAD, MAD, MIR or Direct Methods. The search model may be left intact, although side-chains could be truncated to C γ or to C β using CHAINSAW or PDBSET, respectively (software available within the CCP4 package). Typical MR strategies first involve a rotational search followed by a translational search of the model to correctly orient within a new unit cell. The conventions of the rotation and translation functions were explained in detail.

Candidate solutions can be evaluated for consistency with the data either using Patterson methods or Maximum Likelihood statistics. A final check can then be carried out to prove that there are no steric clashes or overlaps between symmetry equivalents. The success of the transplant is highly dependent on the degree of similarity between the model and the structure, and on the resolution of the data. Success is marked by an easy progression to refinement and appropriate validation statistics.

Chantal Abergel (Information Génomique & Structurale, CNRS, Marseille, FR) presented "Molecular Replacement trick or treat." She opened her talk by pointing out that 70% of the PDB entries made in 2012 (over 8,000) were solved using MR. She then highlighted "requirements" that appear to contribute to obtaining successful MR solutions: the model to target sequence identity should be no less than 20%; the rmsd between model and target should be less than 2 Å; the model should account for approximately 50% of the total scattering material; diffraction data quality and completeness must be good; and the availability of high resolution data is always helpful. The remaining effort in maximising a successful MR outcome lies in optimising the search model, as Dr Abergel described using examples from the Caspr server at <http://www.igs.cnrs-mrs.fr/Caspr2/index.html>. The server enables one to carry out automated MR using homology modelling. Sequence alignment is the first step used to establish domain boundaries. Next, a large number of three-dimensional homology models are generated and then screened in an automated manner for MR solutions using well-established software. Results are reported in hierarchically organized summary sheets for the end user. This approach is certainly attractive for novices in MR and for research programs involving high-throughput structure solution where MR is the method of choice.

The second session focused on techniques for the generation of search models. The first talk was presented by **Marco Marcia** (Yale University, New Haven, CT, USA) and was entitled "Solving nucleic acid structures by molecular replacement." He described the application of molecular replacement in crystallographic structural determination of nucleic acids. The vast majority of the cellular transcripts are non-coding, but the nucleic acid structures that non-coding transcripts adopt are under-represented in the current structural database. Initially it may appear that MR is not well suited for the phase determination of nucleic acids because RNA sequences with even >80% sequence identity may adopt distinct structures. However, Dr Marcia illustrated the utility of MR models for nucleic acid structures of group II introns. He demonstrated that nucleic acid search models tolerate higher rmsd's than such protein models do (using lysozyme as an example). A suite of software tools for nucleic acid structural prediction was also described. The tools include methods for homology modelling and

generation of idealised segments of RNA. The use of these modelling approaches further emphasised how more varied MR searches are available for the determination of nucleic acid structures compared to those methods currently used for proteins.

In the second talk, "Protein families and structural folds in the post-genomic era" presented by **Marco Punta** (EMBL-European Bioinformatics Institute and the Sanger Institute, Hinxton, Cambridge, UK), the current state of structural coverage of sequences in the databases was described. The number of sequences deposited in databases has risen sharply in recent years (eg, the UniProtKB database increased by more than seven million sequences last year – a 45% increase!). A key observation is that the majority of sequences deposited contain domains that match at least one known protein family such as those described in the Pfam database. A consequence of this high rate of matches within known families is that despite the increase in the number of structures being solved per year, the proportion of new families per new protein structure is decreasing (Figure 1). As 35% of known Pfam families lack structure and a similar percentage of sequences currently lack Pfam descriptions, there is still a need to pursue novel structure determinations. Another challenge relates to the observation that many protein sequences lacking a Pfam description are

predicted to be disordered and these proteins may not be amenable to crystallographic determination.

Generation of *ab initio* models and their use as search models in MR were the focus of the last two talks. **Daniel Rigden** (University of Liverpool, UK) presented "AMPLE, a program to process *ab initio* structure predictions into search models for Molecular Replacement." He pointed out that many characteristics of *ab initio* modelling are compatible with MR, and illustrated this point by describing how numerous *ab initio* models may be used as an ensemble of search models. He then described recent developments in AMPLE (*ab initio* modelling of proteins for molecular replacement) and its use as a pipeline for MR within the CCP4 software suite. The method employed by AMPLE involves a large number of polyaniline models that are then clustered (based upon similar core structures), and further modified if required. AMPLE offers a non-CPU intensive way to model proteins of up to 120 residues, and the success rate is particularly high for proteins with all α -folds.

The final talk of this session was presented by **Frank DiMaio** (University of Washington, Seattle, WA, USA) and entitled "Molecular replacement in Rosetta." Rosetta is a versatile software package for predicting and designing protein structures. In MR a correct solution does not always

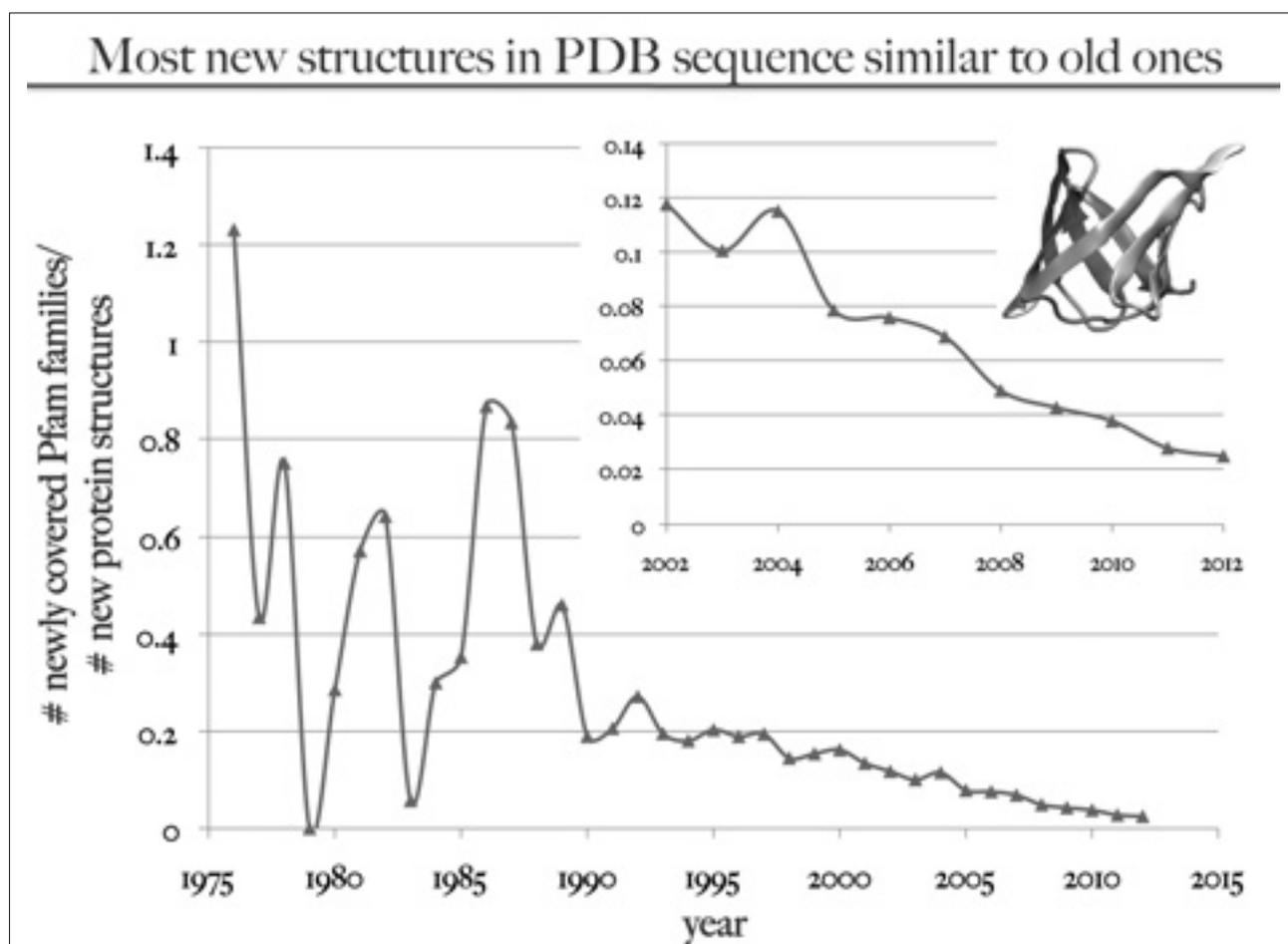


Figure 1: Decreasing numbers of new Pfam families

Over the last 5 years, for every 100 protein structures deposited in the PDB less than 5 Pfam families were newly structurally covered. This indicates that today the vast majority of the proteins for which structures are deposited in the PDB are homologous to proteins previously solved. Note that the ratio reported on the y-axis can be bigger than one as one protein structure can cover more than one Pfam family if constituted of multiple, not-homologous subunits.

result in an interpretable map, particularly in cases where the data are limited in resolution. Rosetta tools were described that enabled refinement of weak molecular replacement solutions. Examples were also given of cases where Rosetta could be used to produce more accurate models from poor quality experimental data. In addition, Rosetta was shown to be a powerful tool for generating high quality *de novo* models using a novel comparative modelling protocol.

Collectively, these talks provided us an opportunity to think about what macromolecules to target in the future with crystallography, and methods for generating effective search models for MR, to solve structures with novel folds and/or limited structural homologies.

The session after tea on Friday began with **Randy Read** (University of Cambridge, UK) presenting “Understanding MR models from single atoms to ribosomes.” He described the newly discovered insight that success with MR in PHASER could be judged with the absolute value of the log-likelihood-gain (LLG) rather than with a relative value. He showed how this has meant that it is possible to use much less data for the initial MR search, speeding up the process considerably. This insight also leads to a better understanding of why fragment-based methods can be so successful, and how these methods can be used to “bootstrap” to full solutions.

Andrey Lebedev (CCP4, STFC Rutherford Appleton Laboratory, UK) presented “Techniques for difficult molecular replacement cases using Molrep and Zanuda.” He discussed the pitfalls of pseudo symmetry, false origins and twinning in MR. He showed, with striking examples, that the program Zanuda can be used to overcome these difficulties to give successful solution with Molrep.

Airlie McCoy (University of Cambridge, UK) used the Star Trek theme to present her talk “Phaser – The Next Generation.” She showed the warp-drive developments in the latest and projected releases of Phaser, including solving the problems associated with translational NCS. She described the modular structure of the program and previewed the changes in the GUI input.

Debora Makino (Max-Planck Institute of Biochemistry, Martinsried, DE) concluded this session with “Structure determination of an RNA-bound 11-subunit yeast exosome complex by molecular replacement.” She described an incredibly challenging project in MR that resulted in the solution of the 400-kDa RNA-bound 11-subunit yeast exosome (Figure 2). The talk illustrated how the difficulties of rapidly decaying crystals were overcome by exhaustive biochemical studies that included the addition of an eleventh

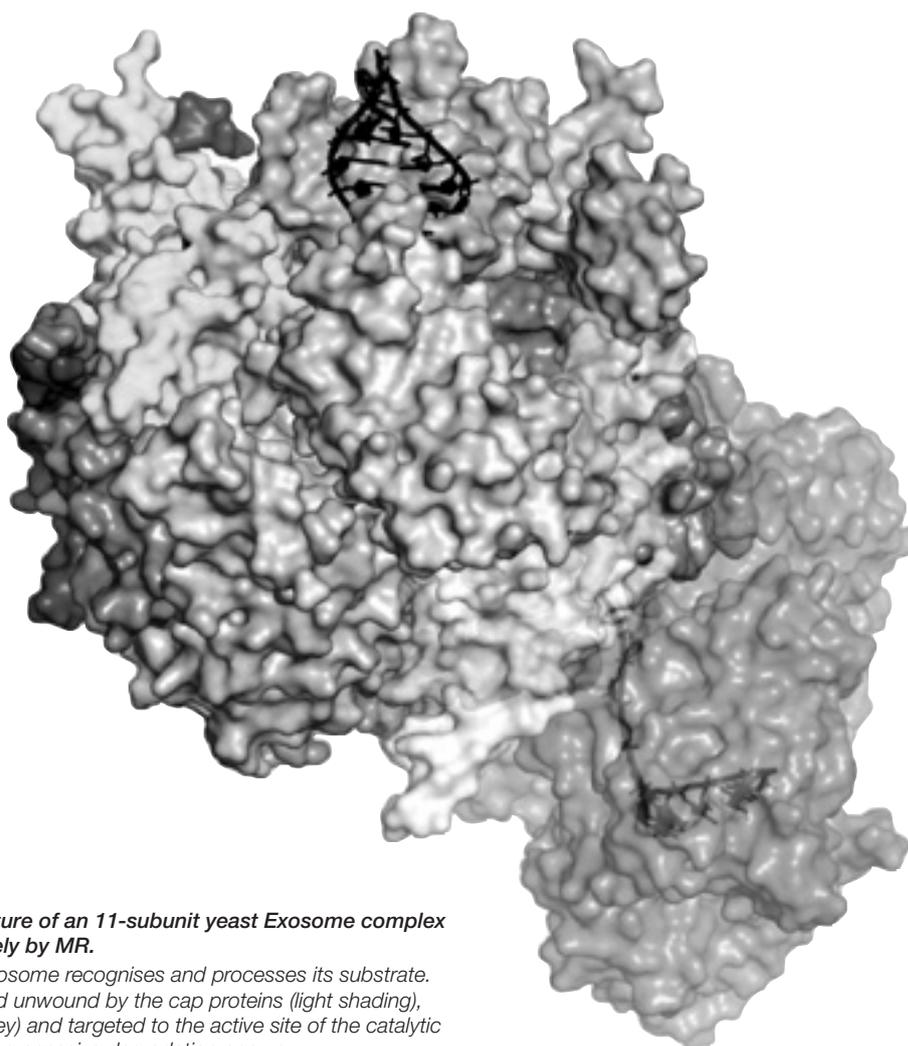


Figure 2: The crystal structure of an 11-subunit yeast Exosome complex bound to RNA solved entirely by MR.

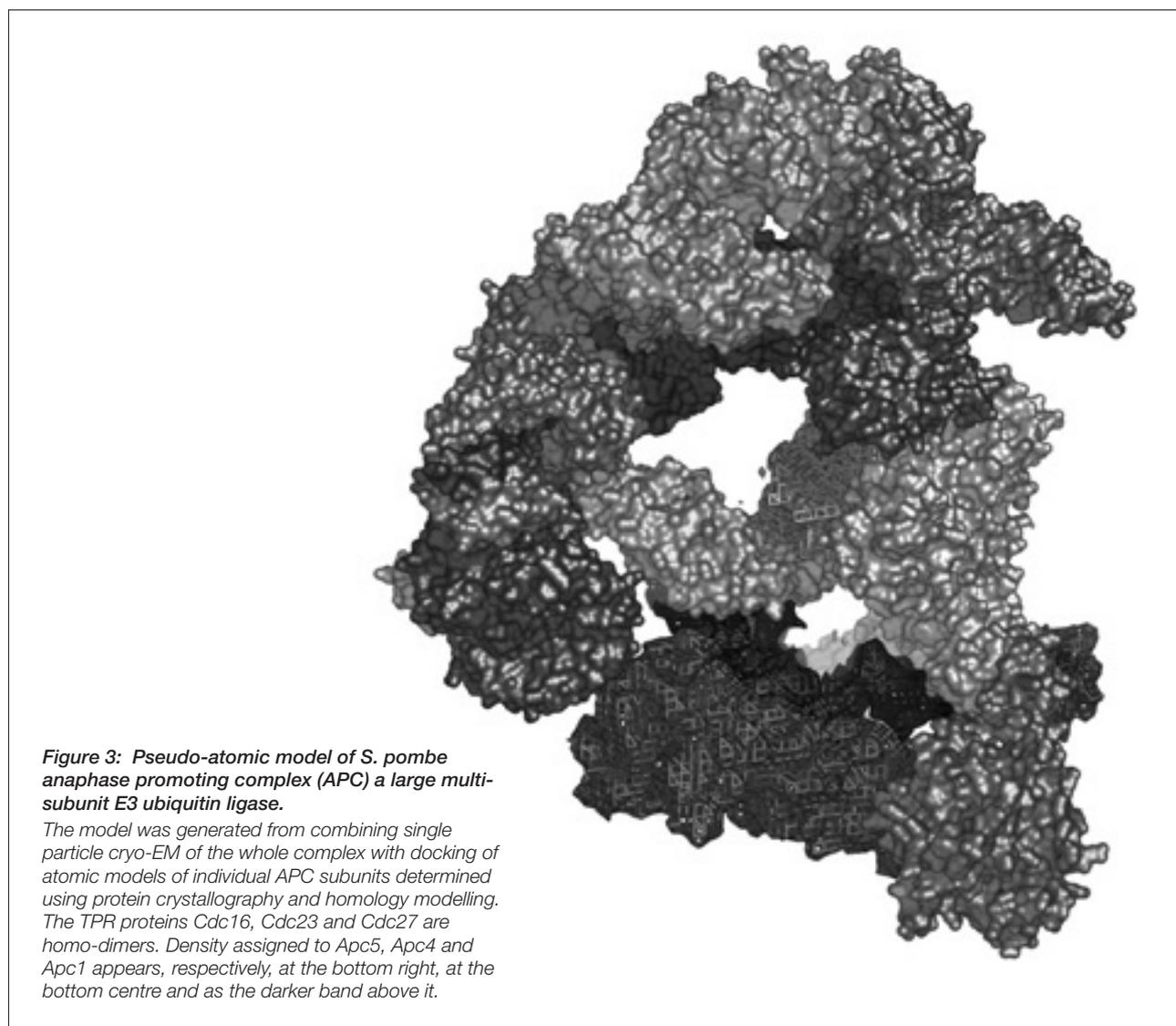
The structure reveals how Exosome recognises and processes its substrate. RNA (black) is recognised and unwound by the cap proteins (light shading), threaded inside the barrel (grey) and targeted to the active site of the catalytic subunit (bottom right), where processive degradation occurs.

protein and an optimized fragment of single-stranded RNA in the crystallization conditions. In spite of sub-optimal search models (lack of homology, low resolution) the exosome structure was successfully solved exclusively by MR. The solution revealed a complex assembly of proteins and helps explain the assembly's multi-functional properties in processing eukaryotic RNA transcripts.

The first session on Saturday morning began with "Determination of a pseudo-atomic structure of the anaphase promoting complex" presented by **David Barford** (Institute of Cancer Research, London, UK). He described a hybrid approach that used crystallography, homology modelling and single particle electron microscopy to position individual proteins within the ~1.2 MDa anaphase promoting complex (APC/C; Figure 3). This complex contains 14 or 15 distinct proteins, some in two copies, and plays a key role in regulating cell cycle events. Baculovirus expression was used to produce APC/C proteins that were then reconstituted as complete or sub-complexes suitable for structural studies. Structural comparisons of different sub-complexes enabled docking of atomic structures or homology models, often by visual inspection, of component proteins within the whole APC/C complex. Technical challenges included the assignment of electron density to a protein with no known

structure and the use of antibody molecules to aid the localisation of specific subunits within the complex. The presentation clearly showed how a "divide and conquer" approach can be used to determine the structures of very large complexes that may not be solved at high resolution using a single technique.

Tom Terwilliger (Los Alamos National Laboratory, Los Alamos, NM, USA) presented the second and final talk of this session, "Using conservation of local structure and connectivity to enhance model-building after molecular replacement." He described a procedure whereby a template structure can be 'morphed' into a more similar target structure first using an electron density map and then with automated model-building to further improve the model. This procedure relies on the assumption that local structures can be superimposed more closely on the target than a model that encompasses the entire target structure. This methodology allows local structural similarities to be maintained but permits global structural changes. Additional improvements to model-building can also be achieved by using this approach to more accurately place models within a unit cell and/or including information about the connectivity within the template being used.



The next session opened with **Andrea Thorn** (University of Cambridge, UK) presenting her talk entitled “SHELXE and molecular replacement.” She told us about how the program SHELXE, more commonly associated with experimental phasing, can be used for molecular replacement. SHELXE is a program for density modification and iterates between DM and backbone rebuilding. The application to molecular replacement comes with the appreciation that the phase information need not come from anomalous scattering. Instead, starting phases from a MR solution can be used. In the case that experimental phases are insufficient, the phase information from MR can be used to bootstrap SAD phase angles. Some useful criteria for success were also given: the resolution of the data should be better than 2.5Å, higher solvent content is better, the estimated value should be as accurate as possible, and finally larger helical content helps – pure β -sheet structures tend to be more difficult to solve.

Nicola Gerardo Abrescia (CIC bioGune – Center for Cooperative Research in Biosciences, Bizkaia, ES) presented “From low to highs: using low resolution models to phase X-ray data.” He illustrated how low phase information obtained from, for example, electron microscopy can be used to phase X-ray data. This was well illustrated by the successful solution of the marine bacteriophage PM2. Some key steps resulting in this success were the correct orientation of the icosahedron using the self-rotation function and positioning of the icosahedron within the unit cell using the translation function followed by real space averaging. A critical experimental consideration is that the resolution ranges of the EM and X-ray data should overlap.

Kevin Cowtan (University of York, UK) concluded this session with “Photoshopping your protein: Model-free refinement.” After molecular replacement, refinement often fails because we are too far from the solution and may be trapped in a local minimum. Challenges may also arise when the search model is not a set of co-ordinates but electron density – we must refine without a model. In order to achieve this refinement a mesh of control points filling the unit cell is used, and search density is distorted onto a target map (calculated from observed magnitudes) by shifting the control points. This was shown to work well, working best for domain-like motions. Future development of this approach may provide an alternative to TLS refinement.

The final session of the meeting was opened by **Giovanna Scapin** (Global Structural Chemistry, Merck & Co., Rahway, NJ, USA) with a talk entitled “Molecular Replacement then and now.” She gave a historic overview and evolution of MR mainly via her personal experiences. She pointed out that 60% of the deposited structures in the PDB have been solved by MR, and that this figure represents a 70% increase in the number of structures solved by this method over the last two years. These structures have been obtained using a number of popular programs, including CNS, AMoRe, Molrep and Phaser, with Phaser showing a substantial increase in usage in recent years. In her presentation, she described a number of challenging MR cases, including the structure solution of p38-MK2 kinase complex.

Gabor Bunkoczi (University of Cambridge, UK) presented “Phaser MRage: automated molecular replacement.” The Phaser.MRage programme starts with a homology search

using the NCBI database. Models are then fed into Phaser for molecular replacement. All models are used and possible solutions are ranked based upon the translation function Z-score. Solutions are also analysed for the presence of possible multimeric assemblies using the point-group symmetry. Phaser.MRage is designed to run efficiently on parallel hardware.

Piotr Sliz (Harvard Medical School, Boston, MA, USA) presented “Wide Search Molecular Replacement – a tool for desperate crystallographers and methods developers.” The WSMR tool is a complete molecular replacement search against ~100,000 protein domains from the SCOP database and can be completed with Phaser within a day using many thousands of processors. He showed that small (less than 12% structural coverage) and low sequence identity (less than 20%) models can be identified through multidimensional molecular replacement scoring metrics. The power of WSMR is demonstrated by a number of examples, including the solution of major histocompatibility complex – T cell receptor assembly by this method.

Andrew C Kruse (Stanford University, Stanford, CA, USA) concluded the meeting with “Applications of molecular replacement to G protein coupled receptors and signalling complexes.” He stated that almost all of the 18 published G protein-coupled receptor (GPCR) structures have been solved using molecular replacement techniques. He first described a commonly employed crystallization technique for membrane proteins using lipid mesophases. Then he discussed the unique aspects of molecular replacement applied to individual GPCRs using crystallization chaperones and fusion proteins. Examples included the solution of the μ -opioid receptor fused to T4 lysozyme.

Finally, this year's CCP4 workshop ran smoothly and successfully due to the dedicated and professional support provided by the UK Science and Technology Facilities Research Council (STFC) team comprised of **Shirley Miller**, **Damian Jones**, **Laura Johnston**, **Karen McIntyre**, **Stuart Eyres** (photography), **Charles Ballard**, and **Ronan Keegan**. In addition, this meeting benefited greatly from the support of the UK-based sponsors: the STFC, the Biotechnology and Biological Sciences Research Council (BBSRC), the Medical Research Council (MRC) and Diamond Light Source.

Prepared by current and past members of the Biological Structures Group Committee and edited by **Katy Brown** (BSG Vice-chairman).



Perception, Passion and Perseverance

Drive and Curiosity: what fuels the passion

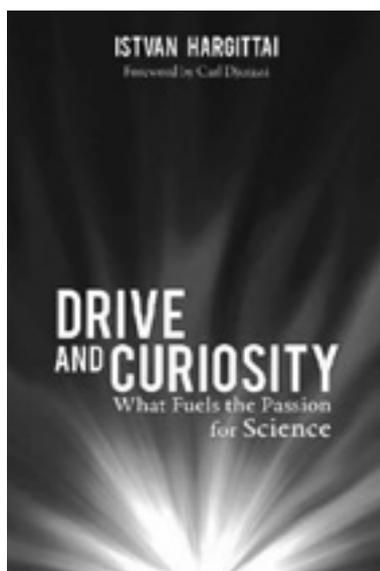
By Istvan Hargittai

Amherst, New York: Prometheus Books, 2011

338 pp

Price 26\$ (hardcover)

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THERE have been a number of attempts to encapsulate the crucial factors that enable a scientist to make a significantly creative rather than a merely incremental discovery. The greater predominance of financial rewards may have led to more emphasis on research aimed at gradual improvements and there is some perception that creativity has decreased by comparison with the mid-20th century. Reflecting on the later 20th century physics, Nobel prizewinner **WA Anderson** regrets both the increased tendency towards quantity over quality in publications and also the reduction in support by government and industry of intellectually exciting research. **Istvan Hargittai**, a respected scientist brought up in Hungary but with wide international experience, has made serious research contributions in symmetry, crystallography and molecular structure. In the past decade or so he has carried out informed relaxed interviews with over 200 Nobel-level scientists and has

written short and longer informal biographies. These have led to 14 books (some jointly with **Magdolna Hargittai**), including six volumes of the *Candid Science* series.

In *Drive and curiosity*, Hargittai has drawn on this experience to select 15 distinguished scientists, mainly chemists or physicists, each of whom represents a character trait that, coupled with drive and curiosity, has led to genuine creativity and discovery in the field of that chapter. Most are well-known and the majority are Nobel prizewinners. One, **Dan Shechtman** representing *Stubbornness*, was even awarded the 2011 Chemistry Nobel (for a discovery in 1982) during publication. Although many achieved success in the USA and a few in Britain, a good proportion were of German or Eastern European extraction, with the scientist or parents leaving because of anti-Jewish discrimination; three were brought up in Hungary. The least familiar is the Romanian/Hungarian combinatorial chemist **Arpad Furka** (born 1931). Coming from a humble farm-worker background in troubled political times, Furka had (like many of the examples) much to overcome; but his technique for peptide synthesis is chosen to illustrate the stimulus of *Saving time and labour*.

In the 1940s and 1950s, women in research had an extra handicap to overcome, not least in the USA, in addition to any personal tragedy. Chemist **Gertrude Elion** (1918-1999) and physicist **Rosalyn Yalow** (1921-2011), who epitomise the themes of *Personal tragedy and Proving oneself* as incentives, each had to surmount poor immigrant backgrounds before encountering academic prejudice. Yalow, who later coped with partial paralysis, began physics research as the only woman in a large engineering faculty. Each woman had a long scientific partnership with a better known male collaborator. Although **Solomon Bersohn** was nominated before his death in 1972, he could not share the Nobel with Yalow when it was actually awarded in 1977. Elion shared the Nobel in 1988 for drug development and treatment with **George Hitchings**, previously her senior in a pharmaceutical lab from 1944. **Rosalind Franklin** (1920-1958), considered in Hargittai's Watson chapter, had an unfriendly relationship with her colleague Wilkins and died before the Nobel was awarded to Crick, Watson and Wilkins in 1962. **Georgina Ferry** has recently outlined the ideal family, location, and education from school to post-doc (in a developing interdisciplinary field) for young women to achieve scientific distinction in the UK; parental support, single-mindedness and stamina are *sine qua non*.

Despite the above, Hargittai chooses the magnetic resonance imaging (MRI) pioneers **Peter Mansfield** (born 1933) and **Paul Lauterbur** (1929-2007) to illustrate the *Overcoming of handicaps* in scientific education. Mansfield trained first as a composer, began his degree at 23 and, through immense drive, graduated Ph D at age 29 while Lauterbur was 33. Military service was a delaying experience for some but

Lauterbur was able to specialize in NMR spectroscopy at a US Army Chemical Center. Active-service experience in Vietnam transformed the aspiration of **Craig Venter** (not described here) towards medically related research. Lauterbur had great difficulty in getting his ideas for zeugmatography, the reconstruction of two-dimensional images, recognized, funded, published or patented, while Mansfield even had to contend with **Raymond Andrew**'s group competing in the same department. The first hint that NMR could be applied medically came from **Raymond Damadian**, who did not receive a share of the MRI prize. As one supported in cancer research, I recall being intrigued around 1971 by reprints of his pioneering NMR relaxation-time tumour-detection papers. Damadian took whole-page newspaper advertisements in Britain and the USA protesting that he should share in the Nobel (although he received other awards).

In the double-helix chapter, **James Watson** (born 1928 into a supportive family) is presented as the 'ignorant' genius, in that his lack of awareness of the limitations of structural chemistry caused him to aim further. His partner, **Francis Crick** (1916-2004), who spent seven years at the British Admiralty on R and D in magnetism, acoustics and electronics before moving towards biophysics is, I feel, an exemplar of collaboration. At successive stages in his career, Crick engaged in fruitful partnerships and so extended his creativity into old age. The right co-worker can fulfill one of Watson's criteria for success: ensure that ideas are exposed to informed criticism. Another example of this is the 2000 Chemistry Nobel for conducting polymers awarded to **Alan Macdiarmid** (1927-2007) together with his younger partners, the entrepreneurial physicist **Alan Heeger** and the polymer chemist **Hideki Shirakawa**. Hargittai uses their achievement to highlight the *Risk to reputation* that Macdiarmid took in moving mid-career from inorganic to unfamiliar organic polymer chemistry.

Sherwood Rowland (1927-2012) has a chapter headed *Reluctant environmentalist* because his first environment-related research exonerated industry by finding that mercury in ocean-going fish was not a consequence of industrial pollution. After realizing with **Mario Molina** that ozone was being removed from the atmosphere he suffered many years as a research outcast, despite being confident of meticulous measurements. They shared the Chemistry Nobel with **Paul Crutzen** in 1995 but Rowland (then aged 68) remained a fairly restrained environmentalist. He had been prompted to investigate chlorofluorocarbons in the atmosphere when he became aware of the measurements of **James Lovelock** who had in the 1950s developed GC detectors (See AS Travis, *RSC Hist Gp N/L*, 2012, **62** 18-25).

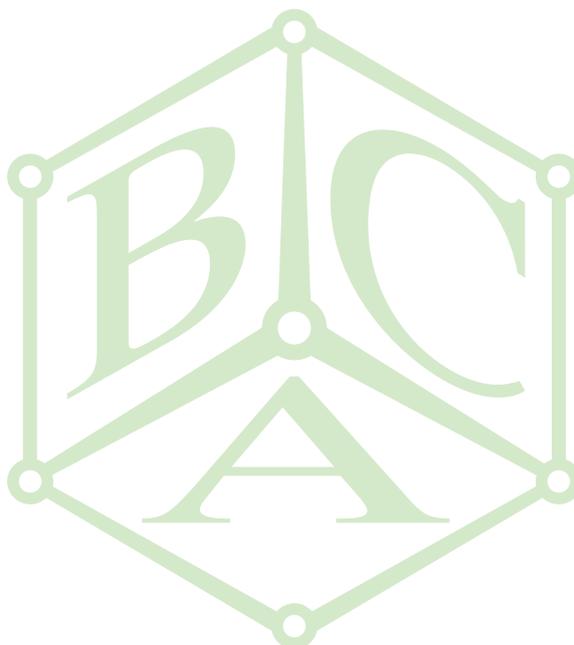
Hargittai's final theme *The joy of understanding* concerns the unorthodox genius **George Gamow**, keen on jokes from his early days in Ukraine and Russia. Despite outstanding contributions to nuclear fusion and astrophysics, including the famous Alpher, Bethe (a contrived non-contributing author) and Gamow paper on the Big Bang, Gamow received few prestigious prizes. Best known for his fine semi-popular books, Gamow did the science that entertained him. Incidentally, **Fred Hoyle**, the steady-state enthusiast who coined the derisive expression Big Bang for what was presumably the ultimate creative event, intended to read Chemistry at Leeds until a scholarship visit lured him to Mathematics at Cambridge.

Hargittai does not pretend that there is a common way for such diverse personalities to achieve outstanding science although most Nobel prizewinners seem to cross conventional disciplinary boundaries. (Lauterbur thought all good research was interdisciplinary.) Obviously, scientific achievers do not all fall into one or other of the 15 chapter types, which include competition (**Linus Pauling**) and beating Nature (**Neil Bartlett**) but not seeking fame. The quiet biochemist **Frederick Sanger** (born 1918) said that possession of two Nobel prizes gave him a secure job! Those who have read any of Hargittai's collections of miniature biographies will doubtless select different representatives and, indeed, make different classifications of motivation. Unusually, the printed pages of this book begin with recommendations from six Nobel Laureates and three other distinguished scientists (with six more on the jacket) and the Foreword, Preface and Introduction by equally eminent scientists are all favourable. In the light of this praise, one can add only that Hargittai's biographical collections generally contain thoughtful insights into the genesis of discoveries that are worth reading; this is no exception.

Derry W Jones
University of Bradford

Reference:

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George Andrew Sim

1929-2012



GEORGE Sim, a pioneer of modern chemical crystallography and the deviser of the Sim-weighted electron density synthesis, familiar to SHELX users as FMAP 5, died in August, 2012.

Born in Aberdeen, Sim began his long association with the Chemistry Department of the University of Glasgow in 1948. After taking an expected First, he joined JM Robertson's X-ray diffraction group in 1952. Within two years he had completed the structures of benzoic acid and $[\text{HO}_2\text{C}(\text{CH}_2)_{10}\text{NH}_3] \text{Br} \cdot 0.5\text{H}_2\text{O}$ and had also convinced his supervisor that he was "a research worker of outstanding brilliance and originality."^{1,2} He then moved to Cochran's group at the Cavendish Laboratory to work on theoretical aspects of the heavy atom method.

Sim did his national service with the Atomic Weapons Establishment at Aldermaston before returning to Glasgow as ICI research fellow. His appointment as lecturer in 1957 ushered in a period of exceptional success in his research. Over the next six years he published roughly a paper a month, the great majority describing three-dimensional structure analyses of important terpenoids, bitter principles, alkaloids and fungal metabolites. This work was recognised by his receipt of the Corday-Morgan Medal and Prize³ for 1963 and of the Fritsche Award for terpenoid chemistry, given to him in 1967 by the American Chemical Society.

By the early 1960s it was clear from the work of Sim and other pioneers both that X-ray analysis could be used as a

routine method of molecular structure determination and that improvements in the design of diffractometers and computers would soon make the technique more accurate and accessible. JM Robertson's 1963 *Presidential Address* to the Chemical Society gives a good picture of the state of contemporary chemical crystallography.⁴

Younger readers should realise that, unlike today when roughly 7×10^5 successful structure analyses have been published, in the early 1960s the number of such analyses was small and each required much hard, tedious and skilled work. Bragg reflexions were recorded on packs of Weissenberg photographs and their intensities were measured by visually comparing them with spots of known relative intensity. Computers and the programs which ran on them were primitive by modern standards – DEUCE which was used for most of Sim's work at this time took 8 – 12 hours for a three-dimensional Fourier calculation and the scale factor had to be punched onto a Hollerith card in Chinese binary. The calculated electron density values were written by hand onto a correctly scaled grid, contour lines drawn and the contours transferred to glass sheets. Sim's ability to filter the correct structure from the noise in a poorly phased map was legendary. Once, when the computer had broken down in the middle of the calculation, he solved a structure with only half the map available.

Sim's interest in the heavy atom method generated a series of theoretical papers which appeared in *Acta Crystallographica* during the late 1950s. The last in the series describes his weighted Fourier technique which makes optimum use of heavy atom phases.⁵ His use of isomorphous replacement to solve the structure of the carcinogenic mycotoxin aflatoxin G1 looks forward to developments in protein crystallography.⁶

In 1964 Sim moved to Urbana to take up a professorship at the University of Illinois. His work there on the alkaloidal tumour inhibitor camptothecin is noticed in the American Chemical Society *Landmarks in Chemical History* series.⁷ His acceptance of a chair at the University of Sussex was quickly followed by a return to Glasgow in 1970 to succeed JM Robertson in the Gardiner Chair of Chemistry. Sim remained in Glasgow till his retirement in 1990. He actively pursued a variety of structural themes: natural product chemistry, conformational studies of nine-, ten- and eleven-membered rings, the stereochemistry of mercury complexes and of metal-carbonyl and -nitrosyl complexes. He also put much effort into the six volumes of the Chemical Society Specialist Periodical Reports on *Molecular Structure by Diffraction Methods*, which he co-edited with **LE Sutton**,⁸ and also his co-editorship of *Acta Crystallographica*. He was a founder member and active supporter of the British Crystallographic Association and he became a Fellow of the Royal Society of Edinburgh.

Sim never lost his love for experimental crystallography. He was not the kind of professor who works exclusively through

the hands of others. Throughout his career he was frequently to be found in the X-ray laboratory, abstractedly humming some favourite classical theme as he worked on a crystal. Shortly before he retired he began to follow order-disorder transitions by studying the effect of changing temperature on crystal structure. Typically, in his derivation of ΔH° and ΔS° values for nitrogen inversion in a 1,3,5-triazacyclohexane from structure analyses at 127, 250, 268 and 293 K, he did all the experimental and computational work himself.⁹

Though Sim was the reverse of pedantic in his approach to experimental science he was quick to spot weaknesses. I remember him appearing suddenly in my office one day to point out gently that my comments on absolute structure in a recent paper were less than satisfactory – this was long before there was a settled approach to these matters. I thought that he behaved in this matter as one would wish a senior colleague to behave – he took the trouble to read one's work and he offered valid comment discreetly. He was equally critical of his own work which he always assessed very soberly.

Two years ago George Sim suffered a stroke from which he did not fully recover. He is survived by his wife Margaret and by his children Kenneth and Linda.

KW Muir

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- 9 G.A. Sim, *J. Chem. Soc., Chem. Commun.*, 1987, 1118 – 1119.

Professor Guy Dodson FRS

1937-2012



GUY Dodson, who died on Christmas Eve 2012, was an inspirational scientist who left an enduring impact on the University of York.

He was born in Palmerston North, New Zealand, twin brother of Maurice to whom he remained very close throughout his life. Guy studied Chemistry in Auckland where he graduated with a PhD in crystallography in 1962. His excitement at the possibilities for structural science encouraged the move to **Dorothy Hodgkin's** laboratory in Oxford. What was

supposed to be a short term post-doctoral position led to him becoming a central figure in her laboratory until Dorothy's retirement in 1976.

His time at Oxford had a defining influence on his life and career. He met and married Eleanor and together they began to establish a scientific reputation and enduring worldwide network through their work on the crystal structure of insulin. Guy also embraced the Hodgkin philosophy of allowing individual talent to mature.

Guy and Eleanor have been a formidable team. Eleanor's mathematical skills have combined gloriously with Guy's enthusiasm for protein structure in making a significant impact across chemistry and biology. Guy moved to York in 1976 as a lecturer in the Chemistry Department and with Eleanor they established a protein structure research group. This was an unusual but visionary appointment by the then head of department, **Dick Norman**, which has had three equally important impacts on the scientific standing of York.

First, there was Guy's personal research when he was at York. Alongside detailed and thoughtful studies of structure and mechanism in systems such as haemoglobin and penicillin acylase, he pioneered effective collaboration with industry, with ground breaking work in protein engineering and structures of insulin derivatives (which are currently multi-billion dollar medicines) and on the structure and mechanism of action of industrial enzymes. This work put York at the centre of the growing field of structural biology, and ideally positioned the laboratory to ride the wave of expansion in the field in the 1980s and 90s. Among many other awards, he was elected as FRS in 1994 and a Fellow of the Academy of Medical Sciences in 2002.

Second, the combination of Guy's passion for structure and Eleanor's leadership in crystallographic methods created the environment which attracted talented scientists to York. Guy mentored a succession of post-doctoral fellows who went on to international prominence in their disciplines. A key quality was his enthusiasm, generosity of spirit and his willingness to devote his time to assist and advise others.

Third, there was Guy's commitment to embedding structural insights into the lexicon of biological research. At York, this was achieved by establishing with **Rod Hubbard** and **Keith Wilson**, the York Structural Biology Laboratory (YSBL) as a research unit within the Department of Chemistry. In 1993, Guy was persuaded to also lead a Division at NIMR in Mill Hill, where his energies established yet another internationally leading research group, bringing structural insights to biomedical research.

Throughout all their time in York, Guy and Eleanor established a serious reputation for hospitality - both for visitors but also for those in difficulties. You never knew who would be staying in the various rooms of the cavernous 101 East Parade - a major party venue for decades.

Guy combined scientific enthusiasm with an impish charm and generated a generosity of spirit in all those around him. He created a laboratory in which there is to this day a real community of scientists who work together for the common good - a wonderful legacy.

Rod Hubbard and Keith Wilson
Department of Chemistry, University of York

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and RSC | Advancing the
Chemical Sciences

Joint BCA/RSC XRF meeting at the University of Leicester, **24th April 2013.**

SPONSORED BY: Bruker, Claisse, PANalytical, SciMed, Specac, SpexCertiPrep and Thermo Scientific.

PROGRAMME

Morning: Sample Preparation Workshop.

09:30 Registration, Coffee and Exhibition.

10:00 Introduction - *Ros Schwarz.*

10:05 Lab session: Grinding, Pressing and Fusion -
Rainer Schramm, Fluxana

11:00 Exhibition & Coffee - Sponsored by Spex Certiprep.

11:30 Lab session: Grinding, Pressing and Fusion -
Frederic Davidts, Socachim.

12:25 Comparative Study between the ISO 9516-1
Standard Method for Analysis of Iron Ore and a
Global Methodology Using Calibration Based on
Certified Reference Materials, *Anne-Catherine
Breton, Claisse*

12:45 Participant sample introduced by *Ros Schwarz.*

13:00 Lunch and Exhibition

Afternoon Presentations.

14:00 Specimen support films - Has Anything
Changed Since 1995? - *Steve Davies,
PANalytical*

14:30 Standardless Analysis with XRF: Where do the
numbers come from and can I trust them? -
Colin Slater, Bruker

15:00 Tea & Exhibition.

15:30 Results from Small Samples - *Nick Marsh,
University of Leicester.*

16:00 Liquid and waste testing - *Gary Smith, Scimed*

16:30 To be advised, *Chris Calam, Thermo*

17:00 Close.

Full details and registration link at: <https://sites.google.com/site/bcaxrf/meetings/24-april-2013>

Meetings of interest

FURTHER information may be obtained from the websites given. If you have news of any meetings to add to the list, please send them to the Editor, c.h.schwalbe@hotmail.com. Assistance from the IUCr website and the *Journal of Applied Crystallography* is gratefully acknowledged.

3-8 March 2013

Glycobiology – Gordon Research Conference, Ventura, CA, USA.

<http://www.grc.org/programs.aspx?year=2013&program=glycobia>

5-14 March 2013

ISIS Practical Neutron Training Course, March 2013, ISIS, Abingdon.

<http://www.isis.stfc.ac.uk/learning/neutron-training-course/>

19-22 March 2013

21st Annual Meeting of the German Crystallographic Society, Freiberg, Germany.

<http://www.conventus.de/dgk2013/>

1-5 April 2013

2013 MRS Spring Meeting and Exhibit, San Francisco, CA, USA.

<http://mrs.org/spring2013/>

4-6 April 2013

Frontiers in Structural Biology of Membrane Proteins, Birmingham, AL, USA.

<http://www.uab.edu/membraneproteins/>

6-14 April 2013

14th BCA/CCG Intensive Teaching School in X-Ray Structure Analysis, Durham.

<http://www.dur.ac.uk/durham.x-ray-school/>

7-11 April 2013

245th ACS National Meeting & Exposition: Chemistry of Energy & Food, New Orleans, LA, USA.

http://portal.acs.org/portal/acs/corg/content?_nfpb=true&_pageLabel=PP_MULTICOLUMN_T5_33&node_id=879&use_sec=false&sec_url_var=region1&__uuid=43fea1e6-e932-43f9-aa36-f4e6769c96da

7-12 April 2013

2nd International School on Aperiodic Crystals, Bayreuth, Germany.

http://old.crystal.uni-bayreuth.de/aperiodic_crystal_school_2013/

8-10 April 2013

Advanced Methods in Integrated Structural Biology of Membrane Proteins – INSERM Workshop 220 Phase 1: Critical Assessment. Bordeaux, France.

10-12 April 2013

Protein Engineering: New Approaches and Applications - A Joint Biochemical Society/Protein Society Conference, Chester.

<http://www.biochemistry.org/Conferences/AllConferences/tabid/379/View/Programme/Page/1/MeetingNo/SA143/Default.aspx>

10-12 April 2013

Understanding Polymorphism & Crystallisation Issues in the Pharmaceutical Industry, Budapest, Hungary.

http://www.scientificupdate.co.uk/training/scheduled-courses/details/171-Understanding%20Polymorphism%20.html?Crystallisation_Issues_in_the_Pharmaceutical_Industry=

10-12 April 2013

Dielectrics 2013, Reading.

<https://www.eventsforce.net/iop/frontend/reg/thome.csp?pageID=116675&eventID=285&eventID=285>

14-16 April 2013

6th "Frolic Goats" High Pressure Diffraction Workshop, Poznan, Poland.

<http://frolicgoats.amu.edu.pl/>

14-19 April 2013

4th Annual Accelerator Reliability Workshop, Clayton, VIC, Australia.

<http://www.synchrotron.org.au/index.php/news/events/australian-events/arw-2013>

15-19 April 2013

EMBO Practical Course: Computational Structural Biology - from Data to Structure to Function, Hamburg Germany.

<http://www.embl-hamburg.de/training/events/2013/CSB13-01/index.html>

16-18 April 2013

Frontiers in Neutron Structural Biology, ORNL, Oak Ridge, TN, USA.

<https://neutrons.ornl.gov/conf/frontier2013/>

18 April 2013

The Physics of Self-Assembling Biopolymers, London.

<http://www.iop.org/events/scientific/conferences/calendar/index.html/?i=1>

20-21 April 2013

TOPAS Users Meeting, Gaithersburg, MD, USA.

[http://www.bruker.com/?&tx_ttnews\[tt_news\]=311&cHash=fd79a9509e33f955a414a209b333457c](http://www.bruker.com/?&tx_ttnews[tt_news]=311&cHash=fd79a9509e33f955a414a209b333457c)

21-24 April 2013

NEUWAVE 2013: 5th Neutron Wavelength Dependent Imaging Workshop, Lund, Sweden.

<http://indico.esss.lu.se/indico/conferenceDisplay.py?ovw=True&confid=45>

21-26 April 2013

Rapid Data Collection and Structure Solving at the NSLS: A Practical Course in Macromolecular X-Ray Diffraction Measurement, Brookhaven National Laboratory, NY, USA.

<http://www.bnl.gov/RapiData/>

22-25 April 2013

APD-IV: Accuracy in Powder Diffraction Meeting, Gaithersburg, MD, USA.

http://www.iucr.org/news/notices/meetings/www.nist.gov/mml/apdiv_conference_2013.cfm

24 April 2013

Joint BCA/RSC XRF Meeting, The University of Leicester.
https://sites.google.com/site/bcaxrf/meetings/24-april-2013?goback=.gde_126033_member_204208200

28-30 April 2013

Intermolecular Interactions in Crystals: Via Experiment and Theory to Industrial Application, Pula, Sardinia, Italy.
<http://www.crs4.it/iic>

29 April - 3 May 2013

Practical X-ray Fluorescence Spectrometry, ICDD, Newtown Square PA, USA.
<http://www.icdd.com/education/xrf.htm>

4-5 May 2013

Chemistry of Supramolecules & Assemblies – Gordon Research Seminar, Les Diablerets, Switzerland.
http://www.grc.org/programs.aspx?year=2013&program=grs_supra

5-10 May 2013

Chemistry of Supramolecules & Assemblies – Gordon Research Conference, Les Diablerets, Switzerland.
<http://www.grc.org/programs.aspx?year=2013&program=supramol>

5-10 May 2013

5th International Conference on Recrystallization and Grain Growth, Sydney, Australia.
<http://www.rex-gg2013.org/>

6-10 May 2013

EMBO Practical Course: Small Angle Neutron and X-ray Scattering from Proteins in Solution, European Photon and Neutron Science Campus, Grenoble, France.
<http://events.embo.org/13-SAXS/index.html>

12-16 May 2013

Nanotech Conference & Expo 2013, Washington, DC, USA.
<http://www.techconnectworld.com/Nanotech2013/>

12-16 May 2013

EMAS 2013: 13th European Workshop, Porto, Portugal.
<http://www.microbeamanalysis.org/emas-2013>

17-22 May 2013

EMBO Conference – The Biology of Molecular Chaperones: From Molecules, Organelles and Cells to Misfolding Diseases, Santa Margherita di Pula, Italy.
<http://events.embo.org/13-chaperone/index.html>

26-29 May 2013

ISDSB2013: 4th International Symposium on Diffraction Structural Biology, Nagoya, Japan.
<http://www.sbsp.jp/ISDSB2013/homepage/index.html>

26-30 May 2013

Nanoscale Pattern Formation at Surfaces, Copenhagen, Denmark.
<http://www.dtu.dk/subsites/nanopatterning2013/English.aspx>

26-31 May 2013

International School on Biological Crystallization – ISBC Granada 2013, Granada, Spain.
<http://isbcgranada.org/>

27-29 May 2013

ESS Science Symposium – Neutrons for Future Energy Strategies, PSI Villigen, Switzerland.
<http://indico.psi.ch/conferenceDisplay.py?confId=2190>

27-31 May 2013

E-MRS 2013 Spring Meeting, Strasbourg, France.
http://www.emrs-strasbourg.com/index.php?option=com_content&task=view&id=569&Itemid=1583

27 May – 15 June 2013

Advanced Methods in Integrated Structural Biology of Membrane Proteins – INSERM Workshop 220 Phase 2: Four Technical Workshops, Grenoble and Paris, France.

30 May – 8 June 2013

Crystallographic Course: The Future of Dynamic Structural Science, Erice, Italy.
<http://www.crystalerice.org/Erice2013/2013.htm>

2-5 June 2013

Next-Generation Organic Photovoltaics, Groningen, The Netherlands.
<http://conference.groningsolar.nl/welcome>

2-7 June 2013

Electron Distribution and Chemical Bonding – Gordon Research Conference, Les Diablerets, Switzerland.
<http://www.grc.org/programs.aspx?year=2013&program=elecldist>

3-6 June 2013

EMU School: Minerals at the Nanoscale, Granada, Spain.
<http://www.ugr.es/~emuschool2013/index.html>

3 June - 13 July 2013

Bachelor Summer Program, Grenoble, France.

9-14 June 2013

Polymers – Gordon Research Conference, South Hadley, MA, USA.
<http://www.grc.org/programs.aspx?year=2013&program=polymers>

9-22 June 2013

The Zürich School of Crystallography 2013, Zürich, Switzerland.
<http://www.oci.uzh.ch/group/pages/linden/zsc/Location.html>

10-14 June 2013

Advanced Methods in X-ray Powder Diffraction, ICDD, Newtown Square, PA, USA.
<http://www.icdd.com/education/xrd.htm>

16-20 June 2013

Workshop on Dynamic Photocrystallography for Chemistry and Materials Science, Buffalo, NY, USA.
<http://www.amercrystalassn.org/photocrystallographyworkshop>

16-21 June 2013

Liquid Crystals – Gordon Research Conference, Biddeford, ME, USA.
<http://www.grc.org/programs.aspx?year=2013&program=liquocryst>

18-21 June 2013

Challenges in Organic Materials & Supramolecular Chemistry, Kyoto Japan.
<http://www.rsc.org/ConferencesAndEvents/ISACS/ISACS10/index.asp>

23-29 June 2013

CRETE13: The 2013 International Conference on Applications of Nuclear Techniques, Crete, Greece.
<http://www.crete13.org/>

24-27 June 2013

15th International Workshop on Physical Characterization of Pharmaceutical Solids (IWPCPS-15), Philadelphia, PA, USA.

24-28 June 2013

4th Workshop on Neutron Scattering Applications in Structural Biology, Oak Ridge National Laboratory, Oak Ridge, TN, USA.

http://www.iucr.org/news/notices/meetings/meeting_2013_58

30 June – 5 July 2013

ICMAT2013 – 7th International Conference on Materials for Advanced Technologies Symposium X: Crystal Engineering of New Materials, Singapore.

<http://www.mrs.org.sg/icmat2013/public.asp?page=home.asp>

30 June – 5 July 2013

Nucleosides, Nucleotides & Oligonucleotides – Gordon Research Conference, Newport, RI, USA.

<http://www.grc.org/programs.aspx?year=2013&program=nucleo>

30 June – 5 July 2013

REI-17: 17th International Conference on Radiation Effects in Insulators, Helsinki, Finland.

<http://rei2013.org/>

1-2 July 2013

South West Structural Biology Consortium meeting, University of Bristol.

<http://www.bris.ac.uk/fmvs/research/swsbc-2013/>

1-5 July 2013

1st International Conference on Tomography of Materials and Structures, Ghent, Belgium.

<http://www.ictms.ugent.be/>

2-5 July 2013

International Workshop on Neutron Optics and Detectors (NOP&D-2013), Munich, Germany.

http://www.iucr.org/news/notices/meetings/meeting_2012_299

2-6 July 2013

International Workshop on Powder & Electron Crystallography, University of Patras, Patras, Greece.

http://www.iucr.org/news/notices/meetings/meeting_2012_406

5-6 July 2013

International Zeolite Pre-Conference Intensive Summer School, Moscow, Russia.

<http://izc17.com/>

7-12 July 2013

17th International Zeolite Conference, Moscow, Russia.

<http://izc17.com/>

6-7 July 2013

Thin Film & Crystal Growth Mechanisms - Gordon Research Seminar, Biddeford, ME, USA.

http://www.grc.org/programs.aspx?year=2013&program=grs_thin

7-12 July 2013

Thin Film & Crystal Growth Mechanisms – Gordon Research Conference, Biddeford, ME, USA.

<http://www.grc.org/programs.aspx?year=2013&program=thinfilm>

8-11 July 2013

11th International Conference on Materials Chemistry (MC11), Warwick.

<http://www.rsc.org/ConferencesAndEvents/RSCConferences/MC11/index.asp>

8-12 July 2013

International Conference on Neutron Scattering, Edinburgh.

<http://www.icns2013.org/home>

13-17 July 2013

9th European Biophysics Congress, Lisbon, Portugal.

<http://www.ebsa2013.org/>

13-18 July 2013

VUVX2013: 38th International Conference on Vacuum Ultraviolet and X-ray Radiation Physics, Hefei, Anhui, China.

<http://vuvx2013.ustc.edu.cn/dct/page/1>

14-19 July 2013

Enzymes, Coenzymes & Metabolic Pathways – Gordon Research Conference, Waterville Valley, NH, USA.

<http://www.grc.org/programs.aspx?year=2013&program=enzymes>

15-19 July 2013

REXS 2013 – Workshop on Resonant Elastic X-ray Scattering in Condensed Matter, Oxford.

<http://www.rexs2013.org/>

20-24 July 2013

2013 American Crystallographic Association Meeting, Honolulu, HI, USA.

<http://www.americalcrystallography.org/2013-meeting-homepage>

23-26 July 2013

Challenges in Chemical Biology (ISACS11), Boston, MA, USA.

<http://www.rsc.org/ConferencesAndEvents/ISACS/ISACS11/index.asp>

2-7 August 2013

SYMMETRY FESTIVAL 2013, Delft, The Netherlands.

<http://symmetry.hu/festival2013.html>

3-4 August 2013

X-Ray Science - Gordon Research Seminar, Easton, MA, USA.

http://www.grc.org/programs.aspx?year=2013&program=grs_xray

4-9 August 2013

X-Ray Science – Gordon Research Conference, Easton, MA, USA.

<http://www.grc.org/programs.aspx?year=2013&program=xray>

3-4 August 2013

Clusters, Nanocrystals and Nanostructures – Gordon Research Seminar, South Hadley, MA, USA.

http://www.grc.org/programs.aspx?year=2013&program=grs_clust

4-9 August 2013

Clusters, Nanocrystals and Nanostructures – Gordon Research Conference, South Hadley, MA, USA.

<http://www.grc.org/programs.aspx?year=2013&program=clusters>

4-9 August 2013

Advanced Neutron and Synchrotron Studies of Materials, Waikoloa, HI, USA.

<http://www.tms.org/meetings/specialty/pricm8/home.aspx>

4-10 August 2013

ISSCG-15. 15th Summer School on Crystal Growth, Gdansk, Poland.

<http://science24.com/event/isscg15/>

5-9 August 2013

62nd Annual Denver X-ray Conference (DXC2013), Westminster, CO, USA.

<http://www.dxcicdd.com/13/index.htm>

11-16 August 2013

ICCGE-17. 17th International Conference on Crystal Growth and Epitaxy, Warsaw, Poland.

<http://science24.com/event/iccge17/>

11-16 August 2013

Nanoporous Materials & Their Applications – Gordon Research Conference, Holderness, NH, USA.

<http://www.grc.org/programs.aspx?year=2013&program=nanopor>

11-16 August 2013

XXII International Materials Research Congress, Cancun, Mexico.

<http://www.mrs.org/imrc2013/>

18-23 August 2013

ICANS25: The 25th International Conference on Amorphous and Nanocrystalline Semiconductors, Toronto, Ontario Canada.

<http://www.icans25.org/index.shtml>

25-29 August 2013

28th European Crystallographic Meeting, University of Warwick.

<http://www.crystallography.org.uk/>

29 August – 1 September 2013

International Conference on Structural Genomics 2013 “Structural Life Science”, Sapporo, Japan.

<http://www.c-linkage.co.jp/CSG2013/>

1-6 September 2013

12th International Conference on Quasicrystals, Kraków, Poland.

<http://www.icq12.fis.agh.edu.pl/>

2-6 September 2013

ICXOM22: 22nd International Congress on X-ray Optics and Microanalysis, Hamburg, Germany.

<http://www.icxom22.de/>

3-6 September 2013

Challenges in Chemical Renewable Energy (ISACS12), Cambridge.

<http://www.rsc.org/ConferencesAndEvents/ISACS/ISA-CS12/index.asp>

8-11 September 2013

11th International Conference on Biology and Synchrotron Radiation (BSR), Hamburg, Germany.

http://www.nature.com/natureevents/science/events/17286-11th_International_Conference_on_Biology_and_Synchrotron_Radiation_BSR

16-20 September 2013

X-ray Free Electron Laser School and Symposium, Dinard, France.

<http://xfel2013.univ-rennes1.fr/>

20 September 2013

X-ray Fundamental Parameters for Reference-Free Analysis, Tsukuba, Japan.

http://www.exsa.hu/news/?page_id=430

23-27 September 2013

15th International Conference on Total Reflection X-Ray Fluorescence Analysis and Related Methods, and the 49th Annual Conference on X-Ray Chemical Analysis (TXRF2013), Osaka, Japan.

<http://www.a-chem.eng.osaka-cu.ac.jp/txrf2013/>

27 September – 1 October 2013

III International Conference on Crystallogenes and Mineralogy, Novosibirsk Russia.

<http://km.igm.nsc.ru/>

30 September – 2 October 2013

Basic Rietveld Refinement & Indexing, ICDD, Newtown Square PA, USA.

<http://www.icdd.com/education/rietveld-workshop.htm>

3-4 October 2013

Advanced Rietveld Refinement & Indexing, ICDD, Newtown Square PA, USA.

<http://www.icdd.com/education/rietveld-workshop.htm>

14-29 October 2013

X-ray Methods in Structural Biology, Cold Spring Harbor, NY, USA.

14-17 October 2013

Myofibrillar Z-disk Structure and Dynamics, Hamburg, Germany.

<http://www.embl-hamburg.de/training/events/2013/SSS13-01/index.html>

15-17 October 2013

Handheld XRF Workshop, ICDD, Newtown Square PA, USA.

<http://www.icdd.com/education/handheld-xrf-workshop.htm>

1-6 December 2013

2013 MRS Fall Meeting and Exhibit, Boston, MA, USA.

<http://www.mrs.org/fall2013/>

2-6 December 2013

Thermec 2013: Neutron Scattering & X-Ray Studies for the Advancement of Materials, Las Vegas, NV, USA.

<http://www.thermec.org/template3s/>

7-11 July 2014

International Conference on Highly Frustrated Magnetism 2014, Cambridge.

<http://hfm2014.tcm.phy.cam.ac.uk/>

5-12 August 2014

IUCr2014. 23rd Congress and General Assembly, Montreal, Quebec, Canada.

<http://www.iucr2014.org/>

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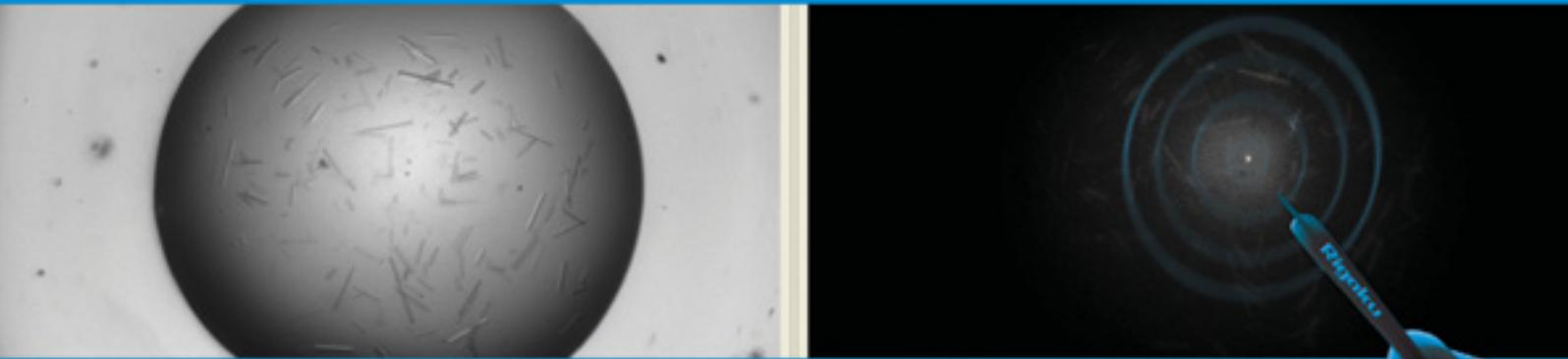
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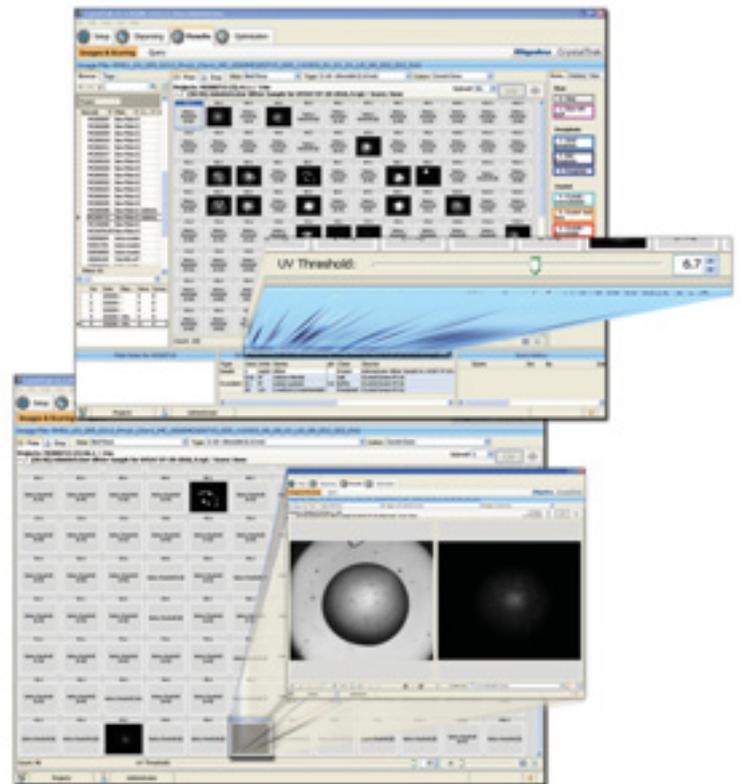
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