

INTERNATIONAL UNION OF CRYSTALLOGRAPHY

IUCr Newsletter

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Original article text and available illustrations

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LETTER FROM THE PRESIDENT

What is Crystallography?

Sven Lidin



Crystallography is the science that develops our abilities to extract structural information using crystallographic techniques. In order to do so, we need to grow crystals, to measure and calculate the properties of crystals and many other things, as well as to perform diffraction experiments. Crystallography thus naturally encompasses much more than the practice and theory of diffraction studies and we need to keep open minds about what should be included in the definition of our science. The discussion is alive and well and we may agree or disagree on whether or not a particular question or technique is crystallography or not and these are important questions: if we fail to recognize a development that is important to our science as being crystallography, we are running the risk of marginalizing our subject, but if we are too inclusive the meaning of the term crystallography is diluted. This is why we need to develop a strategy for the IUCr to cope better with the changes that affect our science as a result of the very development of that science itself and the concurrent development of neighbouring areas. The future of crystallography and the future of the IUCr depends on our ability to cope with change. The scope of crystallography changes and it is a sign of the good health of our subject that it does.

A rather different, but related and certainly equally important question is: what is the relationship between Crystallography the Science and Crystallography the Technique? The question is relevant, because Crystallography is both. We may argue that structural solution is a technique and that Crystallography is the science that underpins that technique, but that is not how the term is used in the larger scientific community. There is nothing strange or unusual about this. Much of the mathematics used in science is not Mathematics the Science, but Mathematics the Technique, commonly referred to

as calculation. No one objects to Mathematics being in the timetable in primary schools, although it is quite obvious that addition exercises and multiplication tables have little to do with the modern development of mathematics. What is important is to instil an understanding that Mathematics the Technique is but a small part of Mathematics the Science.

Similarly, as crystallographers, we need to be clear about the difference between the science and the technique. The latter is based on the former, and when problems applying or understanding the techniques of Crystallography occur, the answers are supplied through the science of Crystallography. You do not necessarily need to understand the subtleties of the science to use the technique, but the risk of making a serious mistake in structural work is much greater if you are unaware of the continuous development of the science.

It may be argued that the science is only necessary for complex and unusual problems, and for run-of-the-mill samples, black-box crystallographic techniques suffice. The fundamental flaw in this argument is that the most difficult problem there is, is to determine whether a problem is difficult or not. Without the science, the technique becomes a cargo-cult enterprise, going through the motions for the sake of protocol. Without the technical use, the science of Crystallography becomes an ivory tower exercise with little impact on the rest of science.

Crystallography remains one of the most successful techniques in all of Science, having made a lasting impact on life and material sciences alike. The great strength of Crystallography is that it provides a standard of performance that few other techniques can offer in terms of reliability, accuracy and reproducibility, but this is thanks to the Science. As the science progresses, it allows the application of the technique to an ever-expanding set of problems and, through this process, Crystallography becomes more important by the day.

As crystallographers we should embrace the interdependence of Crystallography the Science and Crystallography the Technique. This interdependence pushes the boundaries and revitalizes the Science and strengthens the Technique.

EDITORIAL

A bright new future for the IUCr Newsletter

Mike Glazer



For the last 25 years, the *IUCr Newsletter* has been edited and produced in the United States and mainly distributed in hard-copy form. As you will be well aware, the quality of the *Newsletter* owes an enormous amount to the hard work and enthusiasm of its Editor, Bill Duax. Bill and his team in Buffalo have sustained the *Newsletter* all this time from its inception in 1993, and for this the IUCr owes them a huge debt of gratitude. However, Bill has now retired from this post, and we shall certainly miss his attention to detail as well as his many coloured outfits!



Buffalo Bill Duax, Editor of the *IUCr Newsletter* from 1993 to 2017.

The result of this is that for some reason the Executive Committee and the Finance Committee of the IUCr seemed to think that I would be a suitable replacement for Bill. That is going to be very difficult, I know. But with some hesitation, I admit, I agreed to do this, especially when I saw what the IUCr has planned for the future *Newsletter*.

The first thing to note is that the *Newsletter* will be online only, and the guys at Chester have been working hard to create a new fresh look. Of importance from my point of view is that we shall now be able to reach out to a much larger audience around the world, giving us a great opportunity to showcase our subject. For too long, crystallography - despite all its successful contributions to so many Nobel Prizes - has been a rather hidden subject. But the *Newsletter* will open the door to giving us much more publicity, not only to fellow crystallographers and scientists, but also to wider communities including the media, decision makers and professional people in general. We intend over time to make the *Newsletter* as attractive as possible, including dynamic content, such as movies, 3D structures, etc. In order for the IUCr to be able to afford to publish the *Newsletter*, the incorporation of advertising is essential. The ability to include dynamic content should appeal to our advertisers, who can use either static or dynamic images. I hope that all of this will make an attractive publication. You will note too that we have gone for a simple but clear layout, which you can use as a starting page to all other IUCr web pages. If you have any comments on the layout, we shall be pleased to hear from you.

In order to ensure as much international coverage as possible, we have appointed five Regional Editors whose remit will be to report or commission articles from their regions. They are as follows:

Africa: Delia Haynes (dhaynes@sun.ac.za)

Asia: Ted Baker (ted.baker@auckland.ac.nz)

Europe: Serena Tarantino (serenachiara.tarantino@unipv.it)

Latin America: Abel Moreno (amoreno@iquimica.unam.mx)

North America: Amy Sarjeant (sarjeant@ccdc.cam.ac.uk)

For this year we plan to publish two issues and thereafter four times per year as the *Newsletter* develops. We expect that the *Newsletter* will be *the* place to go for finding out news and developments in crystallography.

Finally, let me encourage you to submit contributions for our *Newsletter* to the appropriate Regional Editor, or to myself (Newsletter.Editor@iucr.org) or directly to Andrea Sharpe in the Chester office (newsletter@iucr.org).

As we were going to press, I learnt the sad news that Alexander Moodie has passed away aged 94. Alex - a pioneer in the field of electron microscopy and diffraction - was a Fellow of the Australian Academy of Science and the inaugural winner of the Ewald Prize of the IUCr. His influence on crystallography has been profound and broad, from foundation theories of dynamical scattering to new instrumental developments. An obituary will be published in a future issue of the *Newsletter*.

IUCR JOURNALS NEWS

Andrew Allen appointed as Editor-in-chief of IUCr Journals



We are pleased to announce that Andrew Allen has been appointed as the Editor-in-chief of [IUCr Journals](#). From mid-September 2018, Andrew will be replacing Samar Hasnain, who has completed his six-year term at the helm. We would like to take this opportunity to express our deep appreciation to Samar for his dedicated work and unstinting enthusiasm in developing IUCr Journals, increasing their impact factors, and for launching our flagship journal, [IUCrj](#).

Andrew is a long-time physicist working in materials science, neutron and X-ray scattering at the US Department of Commerce's National Institute of Standards and Technology (NIST), Gaithersburg, MD, USA. His editorial connections with the IUCr extend back to 2002 when he first became a Co-editor of the [Journal of Applied Crystallography](#) (JAC). He became its Deputy Editor in 2011, and one of JAC's Main Editors from 2014. During this time, he has acted as Guest Editor for several JAC special issues. Previously, he has also served on the Editorial Advisory Board of the *Journal of Physics: Condensed Matter* from 1991 to 1996. Andrew's other main connections with the IUCr have centred on the IUCr Commission on Small-Angle Scattering, of which he has been a member or consultant since 2002, and Chair from 2011 to 2014, the triennial conferences on small-angle scattering (SAS), where he has been active on several organizational or advisory committees, including microsymposia organization and other SAS-related activities, at most triennial IUCr Congresses since 1996 (Seattle). He had already agreed to serve on the International Programme Committee for the IUCr2020 Congress in Prague. Previously, Andrew has served as Vice-Chair and Chair of the ACA's Special Interest Group on SAS in 2000 and 2001.

Andrew's PhD research between 1978 and 1981 was under the supervision of Keith Ross at the University of Birmingham, UK, working on the development and application of image-based small-angle neutron scattering (SANS) methods primarily for the microstructure characterization of nickel-based superalloys. Andrew then joined the UKAEA Harwell Laboratory, and his work focused on the development of neutron-based scattering and diffraction materials characterization methods for industrial applications. In this connection, he was a co-author in 1981 of the first research paper on neutron diffraction residual stress measurements. During his time at Harwell, Andrew applied neutron scattering methods, mainly SANS and neutron diffraction, to address a broad range of industrial materials problems, and he started what has become a lifetime research interest in the fundamentals of cement hydration. During a 1988-1989 sabbatical at Northwestern University, Evanston, IL, USA, focused mainly on neutron-based studies of precipitation phenomena in ultra-high strength steels, Andrew was introduced both to the capabilities of X-ray synchrotron facilities and to his future home institute: NIST.

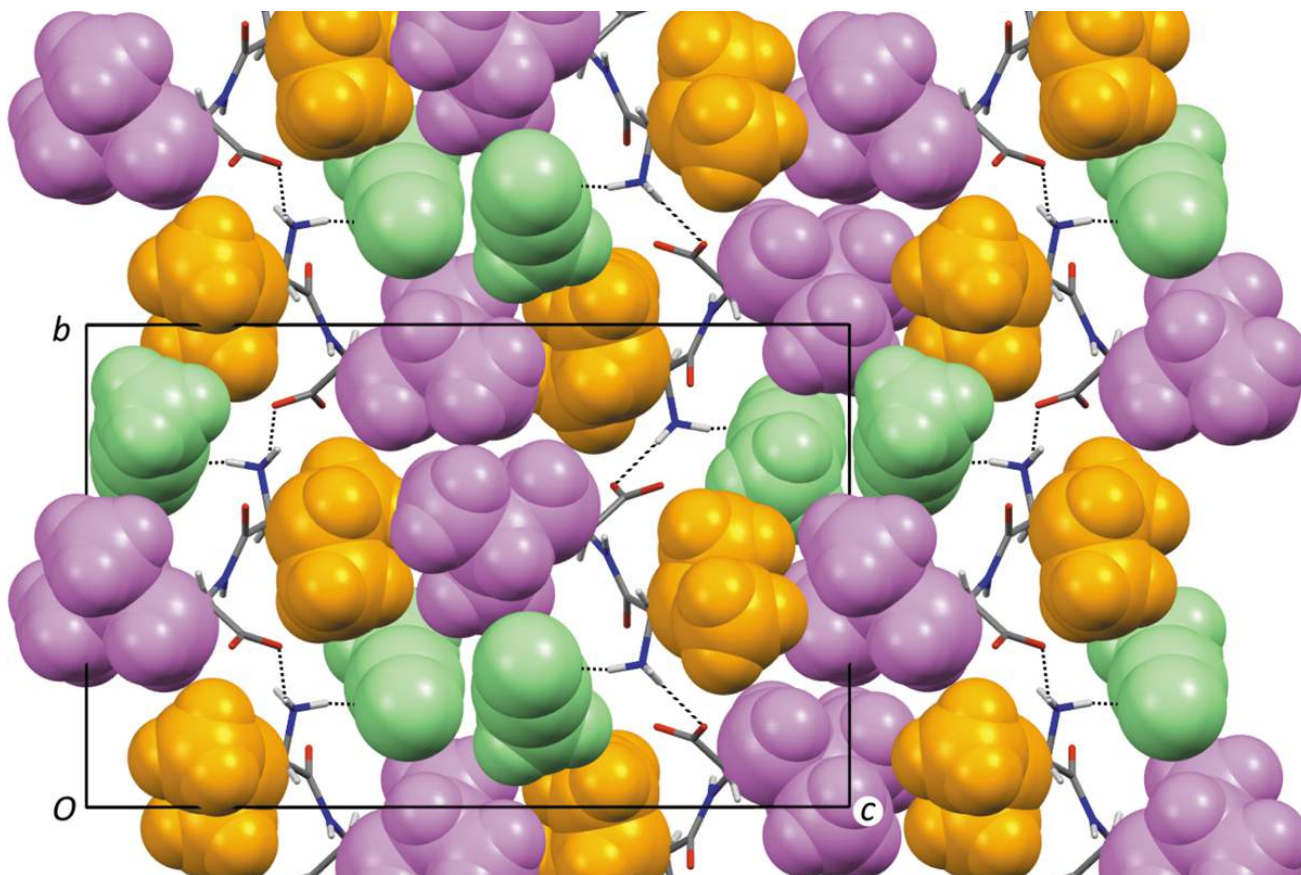
In 1991, initially through a collaboration with the University of Maryland, College Park, MD, USA, Andrew moved to the USA and has been at NIST ever since. At NIST, Andrew has concentrated on microstructural research on advanced materials in support of US Government programmes and industry, together with the development and application of novel neutron and X-ray scattering methods needed for these studies. Among these has been the development and extension of a theoretical formalism for multiple SANS (MSANS) and the development of rapid combined ultra-small-angle X-ray scattering (USAXS), small- and wide-angle X-ray scattering (SAXS and WAXS) capabilities at the US Department of Energy's Advanced Photon Source (APS) at Argonne National Laboratory, IL, USA. Andrew's work has included extensive microstructure-based research on ceramic coatings, porous ceramics, cement hydration and particulate systems, fuel cell materials, nanoparticle systems for biomedical applications, environmental health and safety, porous sorbent materials (including metal-organic frameworks but also porous rocks) for selective gas adsorption, and additive manufactured alloys. These studies have involved SAXS and SANS, neutron and X-ray diffraction studies of heterogeneous materials, as well as X-ray photon correlation spectroscopy (XPCS) for studies of material dynamics. Another component has been SAXS measurements and documentation for new NIST Reference Materials, especially gold and silver nanoparticle suspensions, and the lead role in certification measurements for the glassy carbon SAXS intensity calibration Standard Reference Material, SRM 3600. Over the years, Andrew has received four US Department of Commerce Awards and, despite not working at an educational institution or at a major facility beamline, he has managed to train some 20 students and postdocs in various crystallographic methods for the characterization of materials and materials phenomena.

Andrew Allen has indicated he feels greatly honoured to be appointed the next Editor-in-chief of IUCr Journals, and in particular to succeed John Helliwell, Gernot Kostorz and Samar Hasnain in this position, all of whom he has had the pleasure to work with during his time as Co-editor, Deputy Editor and Main Editor of *JAC*. As is well known, scientific journal publishing is facing a rapidly changing business environment, but Andrew looks forward to facing these challenges and opportunities over the coming months and years in his new role as Editor-in-chief.

RESEARCH NEWS

Hydrophobic dipeptides: the final piece in the puzzle

Carl Henrik Görbitz

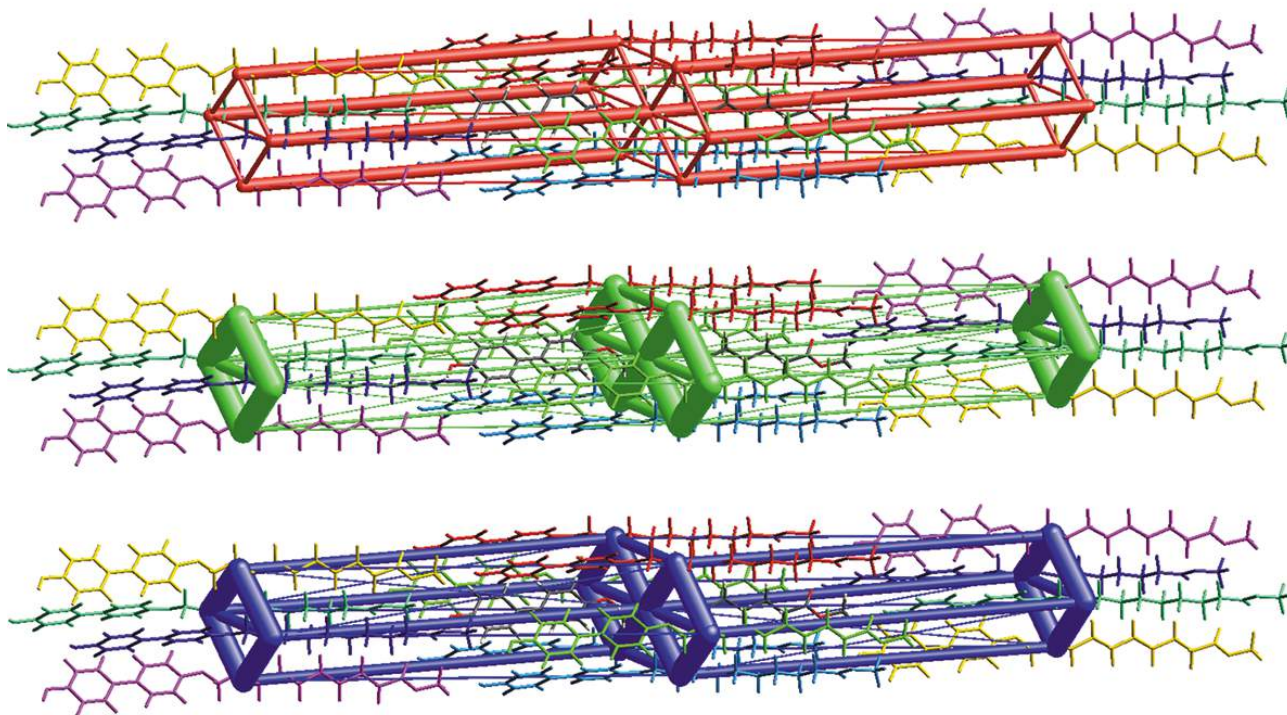


The results from *ab initio* structure prediction programs have demonstrated that any organic molecule has the potential to interrelate with its siblings in a number of different ways, the observed crystal structure representing an energy minimum where the contributions from various types of intermolecular interactions have been carefully balanced. Systematic investigations of molecules that share one important moiety/feature provide valuable experimental data for the understanding of this balance and for rationalizing important trends, even among other sets of compounds. Amino acids constitute an attractive group for such a survey, with a common polar head and a variable side chain. Crystal structures of more than 120 regular acyclic amino acids have been published in the past, meaning that the 20 proteinogenic amino acids represent but a minor fraction of the experimental material. However, if these amino acids are used to construct dipeptides, they alone leave $20 \times 20 = 400$ different options. As of June 2018, crystal structures are only available for 104 of them.

Hydrophobic dipeptides are a subgroup of particular interest. These are based on combinations of the five non-polar amino acids alanine (Ala), valine (Val), isoleucine (Ile), leucine (Leu) and phenylalanine (Phe) only, meaning that hydrogen bonds are essentially limited to connecting the constant parts of the molecules (*i.e.* the peptide main chains). Therefore, any change in the crystal structure upon amino acid substitution can be attributed to the side chain.

The crystal structure of Val-Leu acetonitrile solvate presented in [Görbitz \(2018, *Acta Cryst.* **B74**, 311-318\)](#) is the 25th and final missing piece in the 5 x 5 puzzle of hydrophobic dipeptide structures. This 'completion event' is used as an opportunity to review their crystal packing arrangements and hydrogen-bonding pattern preferences, the associated peptide conformations and the sometimes unexpected impact a seemingly modest amino acid substitution can have not only on the crystal structure but also on the propensity to include co-crystallized solvent molecules.

Special issue on Weak interactions in crystals



Weak interactions have been gaining in importance and interest over the last 20 years owing to their applicability and usefulness in a wide range of scientific disciplines. They are essential in the formation of inclusion compounds, in the self-assembly of host-guest molecular complexes and in the study of polymorphism, co-crystals, phase transitions and charge density.

The [May 2018 issue of *Acta Crystallographica Section E Crystallographic Communications* entitled *Weak interactions in crystals: an integrated approach*](#), explores the fundamental role of detailed structural analysis in understanding weak interactions in the solid state. An [Editorial](#) by Chiara Massera and Helen Stoeckli-Evans introduces this special issue and is followed by a [general review](#) by Andrei Batsanov, which highlights the history, state-of-the-art and future developments of this field. The articles include six research communications on molecular salts, organic compounds and host-guest and coordination complexes. The weak interactions reported have, in many cases, been analysed by a combination of crystallographic analysis and theoretical techniques, showing the importance of an integrated approach. Also, the role of different experimental setups and refinement strategies has been highlighted in an application note.

[Acta E](#) has long been a benchmark for high-quality crystallographic data and structural discussions within the landscape of chemical scientific publications. The rigorous editing and reviewing of the papers, combined with the speed of publication and the open-access editorial policy, makes the journal easily accessible to a very broad audience, encouraging the authors to place their results in a larger scientific context. This is the first special issue that [Acta E](#) has produced and heralds an expansion of the journal's chemical content to highlight hot topics through application notes, themed issues and reviews.

IUCR JOURNALS NEWS

Journal of Applied Crystallography: the first 50 years and beyond



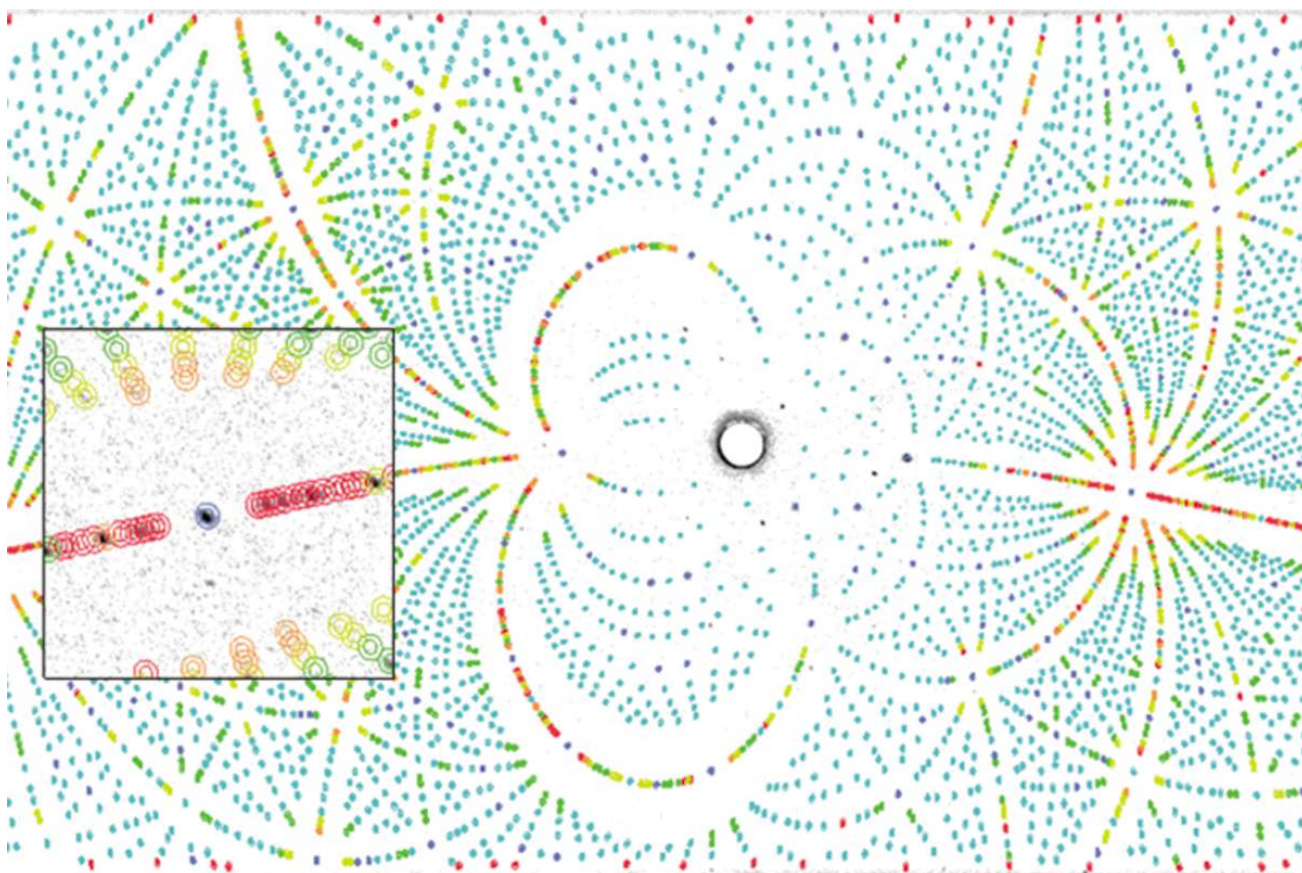
The first issue of *Journal of Applied Crystallography* appeared in April 1968. So, with the April 2018 issue we celebrate its 50th birthday. Although the name suggests a focus on crystallography, *Journal of Applied Crystallography* has served a broad interdisciplinary readership ever since its conception, and the very first paper published was a paper on electron microscopy [Heidenreich, Hess & Ban (1968), *J. Appl. Cryst.* **1**, 1-19]. Before long, *Journal of Applied Crystallography* had developed its reputation as a reliable forum for rigorously reviewed papers across the whole breadth of applied crystallography, with a strong presence of research combining crystallographic methods with other measurements.

Through the hard work of all our editors and editorial staff, *Journal of Applied Crystallography* continues to be recognized as a place to publish significant research featuring applied crystallography and crystallography applied in an interdisciplinary setting, as well as studies on noncrystalline materials. Our mix of published papers continues to include work associated with high-brilliance synchrotron and free-electron laser X-ray sources, despite many other avenues (both IUCr and non-IUCr) being available for reporting such research. We retain a strong presence in neutron scattering applications, and we continue to encourage industrial applications of crystallography. Finally, our founding Editor, André Guinier, would be very pleased to see that the prominence of small-angle scattering, the field he founded, has not diminished in these pages over the years.

We express our appreciation for all the readers, authors, reviewers, editors and technical staff who have made the journal what it has become over the past 50 years. And we look forward to working with the *Journal of Applied Crystallography* community to make the next 50 years even better.

*This is an edited version of the full editorial celebrating the journal's 50th anniversary [Allen, Hajdu & McIntyre (2018), J. Appl. Cryst. **51**, 233-234]. To mark this special occasion, the very first article and the top cited articles from the past 50 years are currently free to read [here](#).*

Special issue on Advanced neutron scattering



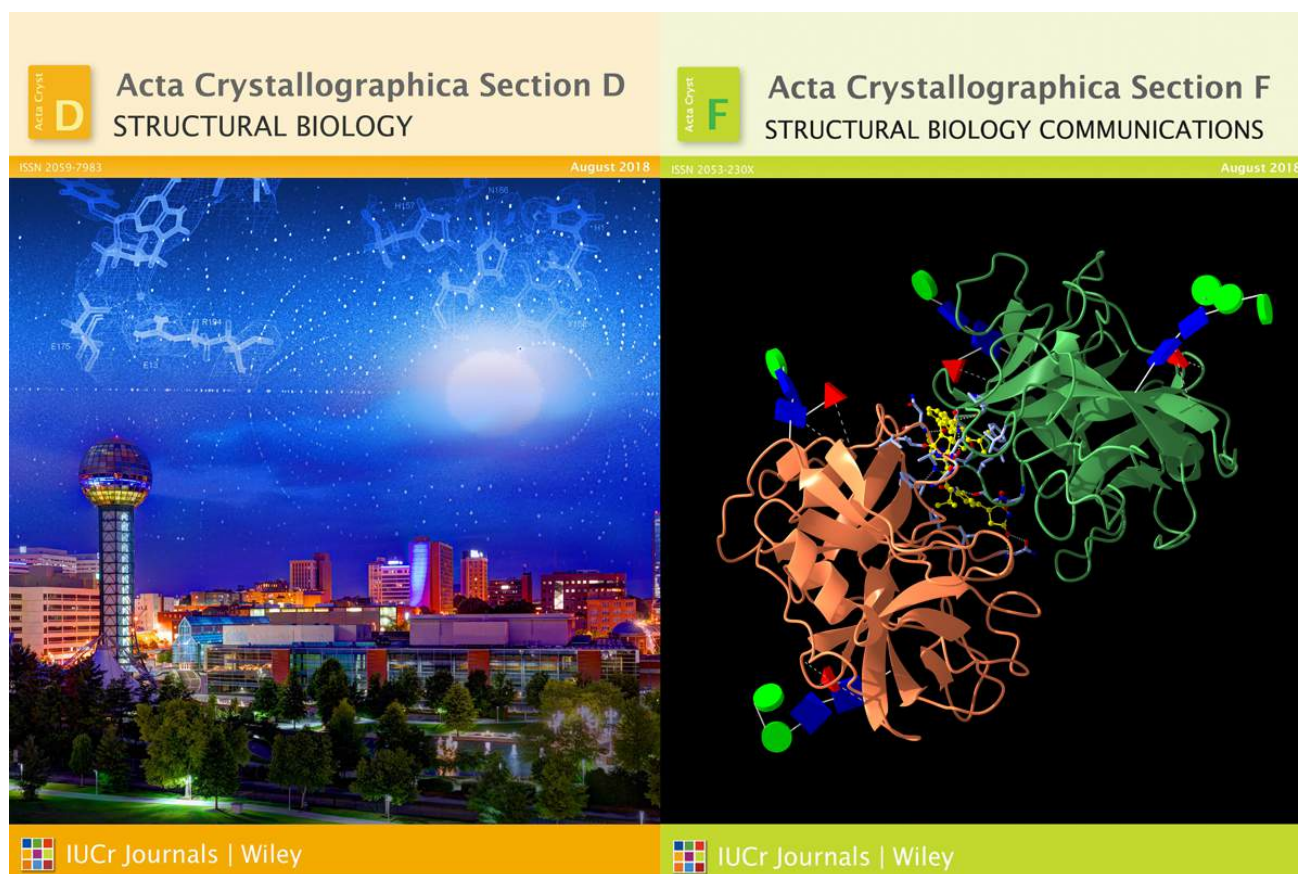
Neutron scattering facilities are called to address an ever-expanding mission in the investigation, development and use of a broad range of materials: from investigating cultural heritage artifacts to advanced bio-materials, from studies of phase transitions and quantum matter to advanced engineering composites for aircraft. This breadth of applications, together with the complex problems they present for making scientific and technical progress, are key drivers for new advanced neutron sources and novel instrumentation that covers an enormously broad scale in both time and space.

These challenges must be met by neutron user facilities within a rapidly changing landscape, and there are significant investments under way in both neutron sources and instrumentation. Some of these developments are highlighted within a new virtual special issue of *Journal of Applied Crystallography* (https://journals.iucr.org/special_issues/2018/ansi/). Europe is constructing the European Spallation Source (ESS), an investment of over two billion USD that is rapidly rising from the ground in Lund, Sweden; the US Department of Energy is investing in the Spallation Neutron Source (SNS) to double its proton beam power on target from 1.4 to 2.8 MW. Both the spallation source at JPARC, Japan, and the SNS are advancing plans for additional target stations. The Institut Laue-Langevin (ILL) is currently executing phase one of its Endurance instrument upgrade program. Both ANSTO's Australian Centre for Neutron Scattering (ACNS) in Sydney, Australia, and the Maier-Leibnitz Zentrum (MLZ) in Munich, Germany, are making significant investments in instrumentation technology and instruments to meet rising user demands.

Within these exciting developments, this special issue on advanced neutron scattering instrumentation highlights some of the innovative advances in neutron scattering instrumentation at facilities around the world that address a broad scientific and industrial scope of applications. The special issue provides us with an opportunity to take a glimpse on a global scale at some of the exciting developments in source and instrument-suite design, high-performance instrumentation, and software. These developments are enabling new opportunities for science discovery through technologies such as detectors, sample environments and data acquisition advances.

This is an edited version of the full foreword to the special issue: [Argyriou, D.N. & Allen, A. \(2018\). *J. Appl. Cryst.* **51**, 567-569.](#)

Two structural biology special issues in IUCr Journals



This August IUCr Journals have published two special issues on structural biology.

Edited by Paul Langan, the [August 2018 issue of *Acta Cryst. D*](#) gives a flavour of the research reported at the 5th International Symposium on Diffraction Structural Biology (ISDSB) held in Knoxville, TN, USA. This meeting brought together researchers from academic and industrial backgrounds and covered X-ray, neutron and electron diffraction, together with complementary techniques such as small-angle scattering, NMR spectroscopy, electron microscopy and advanced computational approaches.

Articles in the issue report recent structural results and describe developments in biological small-angle neutron scattering, X-ray solution scattering and the story of how neutron cryo-crystallography is becoming increasingly popular. The highlights of the first five years of the high-intensity, quasi-Laue neutron crystallography beamline IMAGINE are also reviewed. Finally, there is a discussion of the models determined by neutron diffraction, and improvements to their validation and deposition are proposed.

The [August 2018 issue of *Acta Cryst. F*](#) is dedicated to the crystallography of glycoproteins and protein-carbohydrate complexes. Edited by Jon Agirre and Mark van Raaij, this special issue also has a mix of structural information and cutting-edge methodology. It includes topical reviews on structural and mechanistic aspects of protein *O*-fucosylation, and on using NMR spectroscopy and X-ray crystallography to elucidate protein-glycan interactions in a complementary way.

Our knowledge of the structure of carbohydrates, but especially of their function as post- and co-translational modifications, is now increasing exponentially after perhaps lagging behind that of protein

and nucleic acids. However, there is still some work to do on methodology and this issue presents a number of developments in this area. The issue also reports some recent structures. These include the highly glycosylated human leukocyte elastase in complex with an inhibitor, several enzymes that act on carbohydrates and finally a transcriptional regulator bound to a glycan effector.

IUCR CONGRESS

XXIV IUCr Congress: Microsymposium reports



Instrumentation techniques and/or Computation

MS-085: Dynamic phenomena and material functionality from inelastic X-ray scattering

Chairs: Yoshiharu Sakurai and Eiji Nishibori

This microsymposium covered a wide range of topics in materials science, with a focus on the close relationship between dynamics phenomena and material functionalities. Five speakers, two invited and three contributed, presented recent theoretical or experimental studies on iron-oxo complexes, magnetic multilayers, ionic conductors and lithium-ion battery materials, using inelastic X-ray scattering or inelastic neutron scattering techniques. Each presentation highlighted the importance of these techniques when investigating the spin and electronic states, proton transport and molecular vibration, together with examples of applications to related functional materials. Among them, notable research has been presented by Guo from Carnegie Mellon University, revealing the vibrational signatures of Fe=O moieties in three different oxidation states (Fe^{III} , Fe^{IV} and Fe^{V}). This result, obtained by ^{57}Fe nuclear resonance vibrational spectroscopy, leads to a deeper understanding of the intrinsic reactivity of the Fe=O moiety in iron-oxo complexes. An audience of about 25 joined this microsymposium to exchange ideas and shared a common perspective of inelastic scattering techniques for functional materials research.

MS-086: Accurate high resolution diffraction studies at high pressure

Chairs: Nicola Casati and Krzysztof Woźniak

This is an emerging and broad research field with numerous applications, a number of which were presented during this session. The first speaker, Maxim Bykov (Bayreuth, Germany), presented single-crystal XRD data measured from samples of sizes normally considered to be powders. He and his coworkers synthesized (in DAC under high pressure up to 135 GPa and temperatures up to ca 2700 K) and structurally characterized four novel iron nitrides: Fe_3N_2 , FeN , FeN_2 and FeN_4 . The second speaker was a young student, Yuka Deguchi (Tsukuba, Japan), who presented details of careful multi-temperature (up to 800 K) and pressure (DAC, up to 3.58 GPa) powder studies of charge density for diamond. Next, Boris Zakharov (Novosibirsk, Russia) presented his contribution on the high-pressure studies of the influence of mechanical effects on chemical reactions such as UV or visible light-induced photoisomerisation of Co^{II} complexes and high-pressure dehydration of a series of rare-earth element

hydrated oxalates. The authors related bulk compressibilities, anisotropic lattice strain on hydrostatic compression and associated changes in the atomic coordinates to corresponding transformations upon heating or irradiation by light including high-pressure *in situ* reactions. A very impressive contribution on *in situ* stability of carbonates in the presence of mantle phases was presented by Karen Appel (XFEL, Schenefeld, Germany). Karen and her coworkers studied reactions between Sr and REE-containing carbonates and relevant mantle phases (olivine, enstatite, wadsleyite and perovskite) at high pressure and temperature using synchrotron radiation in a laser-heated diamond anvil cell. Single point XRD patterns recorded during heating allowed them to observe the transformation of the starting silicates to bridgmanite (+ MgO in the cases of olivine and wadsleyite starting materials). The session was concluded by review of experimental possibilities at the newly opened high-pressure diffraction beamline 'XPRESS' at Elettra synchrotron at Trieste presented by Andrea Lausi (Elettra Sincrotrone Trieste, Italy). This session has shown that, although still in its infancy, accurate high resolution studies at high pressure is an emerging field of interesting studies with a wide variety of technical developments and a broad range of new scientific applications.

Materials and minerals

MS-088: Hybrid perovskites

Chair: Roberto Mosca

After the paper by Kim *et al.* in *Sci. Rep.* (2012), lead halide perovskites took center stage in the field of photovoltaics thanks to their excellent performances. However, in the past five years the efficiency race most often prevailed over a definite understanding of the fundamental properties of these materials. Now, while the race is still ongoing, increased attention is being devoted to filling this gap, as confirmed by the lively talks of MS-088. The surface transformation of MAPbBr_3 ($\text{MA} = \text{CH}_3\text{NH}_3$) single crystals exposed to ambient conditions was visualized by M. Banavoth (India), who related the surface restructuring to the photocurrent degradation. On MAPbBr_3 perovskite, A. R. S. Kandada and A. Petrozza (Italy) investigated the recombination dynamics of photo-generated carriers in the frame of a wider study into the role of defects in the photo-excitation dynamics in lead halide perovskites. The use of neutron total scattering and reverse Monte Carlo modelling was used by J. Liu *et al.* (UK) to study phase transitions and reveal local atomic motions in CsPbI_3 and MAPbI_3 , while the interest in CsPbI_3 was confirmed by S. Seth who described the preparation of nanocrystals with different shapes and sizes. Finally, novel hybrids based on the layered perovskite framework were discussed by S. K. Abdel-Aal (Egypt), who reported on materials obtained by alternative alkyl ammonium groups and replacing Pb with Mn, Cu, Co or Bi.

MS-122: Crystallography of materials for energy

Chairs: Oliver Oeckler and Artem Abakumov



Chairs and invited speakers.

This microsymposium showed that the broad spectrum of crystallographic methods can significantly contribute to almost all relevant classes of materials. On the last afternoon of the congress, the microsymposium attracted a large audience and there were more questions than time allowed for answers. The talks were lively and the speakers did not hesitate to call their results 'cool' and 'weird'. Subjects ranged from battery materials and photovoltaics to zeolites for energy storage and nuclear fuels. Most speakers reported on combined methods for structure determination, e.g. neutron and X-ray diffraction in synergy with XAS in order to elucidate disorder in lithium manganese titanates (Siegbert Schmid). TEM methods also played an important role, e.g. concerning the analysis of materials for solar cells (Joke Hadermann).

Physical and/or Fundamental

MS-089: Chemistry and physics of modulated and composite crystals

Chairs: Siegbert Schmid and Thomas Doert



Speakers and chairs (l-r): Somnath Dey, Paul Klar, Siegbert Schmid (Chair), Laura Folkers, Cinthia Corrêa, Thomas Doert (Co-chair), Olivier Perez and Sven Lidin.

Up to 90 attentive listeners gathered to attend six excellent presentations on recent results on modulated and composite crystals. The scope of the microsymposium was deliberately broad and a diversity of chemical systems was discussed, including coordination compounds, silicate minerals, tungsten bronzes and intermetallic phases. A special highlight was the presentation by Sven Lidin, just prior to his election as President of the IUCr, who presented recent results on the structural dynamics of intermetallic systems at moderate temperatures. In an impressive and captivating talk, he showed that incommensurate structures often occur as intermediates between disordered high-temperature and ordered low-temperature phases in intermetallic systems. In a novel and highly thrilling series of synchrotron X-ray diffraction experiments he was able to follow the segregation of binary intermetallic phases *in situ*, providing new insight into the reaction mechanism as well as its dynamics. Thanks to experienced, enthusiastic but also disciplined speakers and well prepared presentations, all talks were followed by vivid discussions, appreciated by the speakers and audience alike.

Special Activities

MS-095: Crystallography for space sciences

Chairs: Juan Manuel Garcia-Ruiz and Hanna Dabkowska



Speakers.

This was the first meeting devoted to *crystallography in space*, proposed as a follow-up to the very successful COSPAR-IUCr workshop organised in Puebla, Mexico, in 2016 (<http://www.inaoep.mx/cospar2016/>). There were five excellent presentations: mineralogical results from the Mars Science Laboratory Rover Curiosity by David Blake (USA); mineralogy and crystallography of samples returned from primitive asteroids by Tomoki Nakamura (Japan); prospects for organic minerals on Saturn's moon Titan by Helen Maynard-Casely (Australia); early stages of grain formation studied by microgravity experiments by Yuki Kimura (Japan); and ordering phenomena in minerals: verve phase of natural magnetite by Giuditta Perversi (UK). Dominique Maez (Belgium) gave a short presentation about the influence of microgravity on the diffraction properties of protein crystals. The session was so well attended that there was no room to sit, and the subsequent question-and-answer period with animated informal discussion lasted about an hour after the end of the time provided. One of the discussion topics was whether a Crystallography in Space Science Commission (CSSC) would be a good addition to the IUCr. There was a lot of support for this idea and the proposal for such a commission will probably be presented at the Prague congress, after more discussion with the scientists involved.

IUCR CONGRESS

XXIV IUCr Congress: Satellite meeting reports



Phasing and model building

Organizers: Mangayarkarasi Nivaskumar and Anthony Addlagatta

As India hosted its first ever IUCr Congress from 21 to 28 August 2017, Anthony Addlagatta and I, as organizers of the satellite meeting Phasing and Model Building, proudly claim to have left no stone unturned. The 1.5 day meeting had lectures and tutorials on relevant subjects and took place with the cordial hospitality provided by S. Chandrashekar, the Director of the Indian Institute of Chemical Technology (IICT), Hyderabad, at the premises of the Centre for Chemical Biology. We thank him immensely; without his support it would not have been possible to make this event a *no registration fee* meeting for all our participants.



We also thank Tom Terwilliger (Los Alamos National Laboratory, USA) and Charles Ballard (STFC Rutherford Appleton Laboratory, UK) who promptly and enthusiastically accepted our invitation to organize such an event and came up with a programme and suggestions for the tutor team. We had Eleanor Dodson (University of York, UK), Hung Li-Wei (Los Alamos National Laboratory, USA), Dorothee Leibschnner (Lawrence Berkeley National Laboratory, USA), Claudia Milan Nebot (Molecular Biology Institute of Barcelona, Spain), Felix Simkovic (University of Liverpool, UK) and Sravya Mounika Kantemneni (EMBL Hamburg, Germany) as tutors, a good scientific mix from the USA and Europe. Together, we had a package of molecular replacement, *CCP4*, *Coot*, phasing methods for X-ray and EM, and tools for model and ligand building for this meeting.

On 20 August, we started with Professor Dodson discussing the essential elements of molecular replacement, followed by Dr Terwilliger who gave a lecture on phasing with *PHENIX*. Dr Nebot then discussed a rather new program, *ARCIMBOLDO*, which could be used for fragment-based *ab initio* macromolecular phasing. Dr Simkovic discussed integration of bioinformatics with structure refinement using *MrBUMP*, *AMPLE* and *SIMBAD*. Dr Ballard later lectured on aspects of the *CCP4i2* and *Coot* programs. Dr Leibschnner closed our lecture session with a discussion of Polder maps and their application in improvising ligands with low electron density.

The programme had an equilibrium in terms of the scheduled lectures and break times, which was appreciated by the participants who were recommended to bring their own laptops with the required software installed and also bring any data that they would like the tutors to help them with. Restricting the number of participants to 30 was evidently helpful to facilitate one-to-one discussions throughout the meeting. On the first day, Dr Ballard and Professor Dodson eagerly helped students with tutorials on molecular replacement and *Coot* until around 22:30, after dinner. The morning of the 21st started with Dr Terwilliger discussing phasing in the context of cryoEM, post breakfast. This was followed by Ms Kantamneni's tutorial on new *ARP/wARP* workflows for phasing and model building. The workshop ended with Dr Li-Wei, Dr Terwilliger and Dr Leibschnners' tutorials on various aspects of phasing and the generation of Polder maps.

We had an overwhelming response from many principal investigators (PIs) across India. We had earlier identified little more than 100 PIs involved with protein crystallography in India and sent out invitations encouraging nominations of one student per laboratory. We thank all the PIs for having understood our constraints and complying with us. We extend very many thanks to all participants for the success of the event, exemplified by their positive feedback. If they thought anything could be improved it was more time with the tutors and more modules. We thank all the members of the AA (Anthony Addlagatta) lab for helping us with organizing accommodation, food and logistics. Together, we had a great time learning about methods in phasing and model building, which would not have been possible without the IUCr2017 Congress. We do hope to conduct other meetings and workshops at IICT, which would constructively help the Indian crystallography community to bridge science and expand horizons.

Crystallography and society

Organizer: Ashwini Kumar Nangia

This satellite meeting, which took place at CSIR-NCL, Pune, India, on 29-30 August 2017, addressed issues in the fields of natural and social sciences that concern the countries in and around India.

Gautam Desiraju (Indian Institute of Science, Bengaluru, India) gave a talk entitled 'Science and Society. What do they owe each other?' He began by saying 'Science is objective and scientists should be neutral, impersonal, dispassionate and far from the madding crowd. Scientists will not be concerned with politics if their science is to be pure and environmentally relevant. Science is about real life'. He quoted John

Desmond Bernal's statement, 'Science is an integral part both of material and economic life and of ideas which guide and inspire it'. Desiraju asked whether scientists should be influenced by societal and political pressures that swirl around them. He asserted that scientists should lead society as the custodians of higher values including truth, justice and respect for human diversity and culture. The world is peopled by winners and losers, and scientists are among the winners. We are educated, financially advantaged and have opportunities that are denied to most others. We have the potential to excel in our professions. This privilege comes with a responsibility; scientists owe it to the society around them to provide guidance, leadership and moral stature. They become the role models for others. Desiraju said 'Good science is about morality and ethics'. He talked about the scientific ego or scientific narcissism and how it influences the scientific profession. Concluding his talk he put forward a quote by Nagarjuna, the Mahayana philosopher, who said 'For the sprout does not exist in the seed which is its cause; it does not exist in each one of earth, water, fire, wind and so forth, which are agreed to be its conditions; it does not exist in the combinations of conditions, nor in the combination of causes and conditions, and it does not exist as separate from these, free from causes and conditions'. To then define what the sprout is, is the essence of consciousness, or a lower-level complex phenomenon such as the crystalline state.



Speakers (l-r) Pinak Chakrabarti, Sven Lidin, William L. Duax, Gautam Desiraju and Ashwini Nangia.

William L. Duax (Hauptman Woodward Medical Research Institute, Buffalo, NY, USA) gave a talk on 'Genomics, Crystallography, Bioinformatics, Molecular Evolution, and Drug Design'. He presented information about the International Gene Bank, three billion years of evolution of the sequences of superfamilies of known and hypothetical proteins, and why we need to develop methods to determine the functions of all of the proteins in our environment in order to design drugs without 'side effects'. He talked about proteomics, the determination of a reliable evolutionary tree of all species on earth, and identifying the last universal common ancestor of all cellular species. J. J. Vittal (National University of Singapore) described 'Crystallographic Activities in and around Singapore'. In his talk entitled 'Science gazing, standing on the shoulders of crystals', Pinak Chakrabarti (Bose Institute, Kolkata, India) discussed the theory and practice of crystal growth. He explained how additives induce sodium chloride

morphology modifications and described a practical approach to produce near-spherical common salt crystals with better flow characteristics. He described crystallographic applications in archaeology, forensics, art and drug design. He cited the work of renowned woman crystallographers including Rosalind Franklin, Ada Yonath and Kathleen Lonsdale.

In his talk 'Crystallography and Society in South Africa and throughout Africa', Andreas Roodt (University of the Free State, Bloemfontein, South Africa) discussed the BRICS nations, academic and industrial science, and African initiatives. He discussed applications of crystallography to radiopharmaceuticals, homogenous catalysis, separation technologies and utilization of carbon dioxide. He was optimistic about networking among African scientists. Sven Lidin (Lund University, Sweden) asked 'Does crystallography blind us with its images?', and B. Chandrasekharan (CSIR-Central Leather Research Institute, Chennai, India) threw light on the subject 'Capacity Building in Industrial Research – Emerging Roles of CSIR'. Amitava Das (CSIR-Central Salt and Marine Chemicals Research Institute, Bhavnagar, India) spoke about 'Salt and its opportunities in India'. He discussed sources, large-scale production, availability, consumption, purity and the cost of salt in India. He talked about the future distribution of salt in India and the world. G. Thyagarajan (Zaheer Science Foundation, New Delhi, India) spoke about the 'Science-Based Economic and Social Development: Presenting a Fresh Approach to Reach the Unreached in the Global Society'.

In his closing talk 'Science outreach to society by CSIR-NCL', Ashwini Kumar Nangia described crucial technologies developed by the scientists from CSIR-NCL that benefit society. He cited examples of water filtration units, oxygen enrichment units and immersion of Ganesha idols in an eco-friendly way.

REGIONAL NEWS

Brief history and activities of the Bulgarian Crystallographic Society

Daniela Kovacheva



Participants at NCS2016.

The Bulgarian Crystallographic Society (BCS; <http://www.bgcryst.com/>) was officially registered in Bulgaria in April 2010, and in 2011 applied for membership of the IUCr at its XXII General Assembly and Congress in Madrid, Spain. BCS was officially approved as an individual member (Category I) on 25 August 2011 (<https://www.iucr.org/world/bg>). BCS is also a member of the European Crystallographic Association (ECA).

Following the initiative of the IUCr for proclamation detailing the development of crystallography in South East Europe, BCS responded to the IUCr's request and prepared a summary of the development of crystallography in Bulgaria, which was published in one of the three Crystallography in South-Eastern Europe issues of the *IUCr Newsletter* [*Crystallography in Bulgaria* (2011). **19**(4), 11-14].

Recent activities of the BCS (October 2016–November 2017)

During recent years, the National Crystallographic Symposium has won recognition as a leading scientific event, not only for the Bulgarian crystallographic community but also for participants from different European countries. These Symposia are the principal scientific activity of the BCS and reflect the current state of research in the fields of crystallography, crystal chemistry, crystal physics, mineralogy and materials science, and are thus characterized by an interdisciplinary spirit.

The BCS also organises specialized international and national workshops (supported by the IUCr and ECA) to promote crystallography among young scientists.

Vlth National Crystallographic Symposium

The Vlth National Crystallographic Symposium (NCS2016), held in the Grand Hall of the Bulgarian Academy of Sciences (BAS), Sofia, 5-7 October 2016, was the latest project of an initiative started at the beginning of 2009 by a group of Bulgarian crystallographers/enthusiasts, and is nowadays conducted under the auspices of the BCS. Following the path established during previous Symposia, the organisers - in conjunction with the BCS - have dedicated a special honorary sign to Kostadin Petrov from the Institute of General and Inorganic Chemistry (IGIC)-BAS. Professor Petrov was the first amongst the enthusiasts to start not only thinking about but also take action in establishing an independent crystallographic society in Bulgaria.

The NCS2016 lecturers were leading researchers in their respective fields: Svetlana Mintova (ENSICAEN, France), Katharina Fromm (University of Fribourg, Switzerland), Krzysztof Wozniak (University of Warsaw, Poland), Atul Khanna (Guru Nanak Dev University, India), Srebri Petrov (University of Toronto, Canada), Boriana Mihailova (University of Hamburg, Germany), Evdokiya Salamanova (Karolinska Institute, Stockholm, Sweden), Bogdan Rangelov [Institute of Physical Chemistry (IPC)-BAS], Pavleta Shestakova [Institute of Organic Chemistry with Centre of Phytochemistry (IOCCP)-BAS], Radostina Stoyanova (IGIC-BAS), Yuri Kalvachev [Institute of Mineralogy and Crystallography (IMC)-BAS], Ivanina Sergeeva [Institute of Genetics (IG)-BAS], Alexander Karamanov (IPC-BAS), Liliya Vladislavova (Otto-Schott-Institut für Materialforschung, Friedrich-Schiller-University Jena, Germany), Tzonko Kolev [Institute of Molecular Biology (IMB)-BAS] and Galina Gencheva (Sofia University).

The audience included more than 130 scientists (110 registered) from 7 Bulgarian universities, 16 institutes of the BAS and scientists from universities and institutes in Poland, Switzerland, Germany, France, Sweden, Italy, Slovakia, Spain, Estonia, Turkey, the Republic of Macedonia, Czech Republic, Canada, USA and India. A total of 22 oral and 65 poster presentations involved more than 250 authors. It is worth noting that over 50% of the participants were students, PhD students and young scientists, who actively participated in the poster sessions. The organisers of the National Crystallographic Symposia try to encourage and support the scientific progress of young researchers, and for the second time, the organisers were supported by the Ministry of Science and Education and the Bulgarian National Science Fund through a grant (DPMNF 01/13-27.09.2016) especially targeting the young scientists. Members of the international jury had the difficult task of selecting the best young scientist poster presentation, which was awarded to Mariya Kalapsazova (IGIC-BAS) for presenting 'Diffraction methods for analysis of layered $\text{Na}_x\text{Ni}_{0.5}\text{Mn}_{0.5}\text{O}_2$ as cathode materials'. The Symposium attracted the attention of several different Bulgarian official institutions: the Deputy Chairman of the Bulgarian Parliament, Ivan Ivanov; members of the Parliament's Commissions for 'Education and Science', 'Children, Youths and Sports' and 'Environment and Water'; Parliament's Deputy Chairpersons, Borislav Velikov and Vili Lilkov; the Minister of Education and Science, Meglena Kuneva; the Rector of the University Chemical Technology and Metallurgy, Mitko Georgiev; and the President of BAS, represented by the Vice President Corresponding Member, Nikolay Miloshev.

National workshop: Introduction to Powder X-ray Diffraction (IPXRD-2017)

This national workshop was conducted in the University Chemical Technology and Metallurgy in Sofia from 19 to 23 June 2017. It was organized by BCS with the active support of IGIC-BAS, the Institute of Mineralogy and Crystallography (IMC)-BAS, the Geological Institute-BAS, the Faculty of Geology and Geography of Sofia University 'St Kliment Ohridski', and the University of Chemical Technology and Metallurgy (Sofia). Predominantly young researchers comprised the 37 registered participants from Sofia, Plovdiv, Varna and other Bulgarian towns. Most of the participants were from the academic community

(BAS, universities and museums) with a wide range of competence, from students up to associated professors and full professors. Interest was also shown by business and trade companies, namely Kaolin EAD (Senovo), Evrotest-Control (Sofia), Travel Management (Sofia) and Sensata Technologies Bulgaria Ltd (Sofia).

A cycle of lectures gave the participants basic knowledge of the crystallographic description of solid substances, the features of the X-ray beam and the principles of its use for analyses of powder materials. The exercises during the workshop were directed not only to the young researchers but also to specialists from companies with activities in the field of material science. Items discussed included how to use X-ray diffraction for the identification of crystalline phases and mixture of phases and how to obtain the maximum information from them: indexation of powder patterns, symmetry and unit-cell parameters, quantitative relations between phases, crystallite size and morphology determinations.



Participants at IPXRD-2017.

The lecturers shared their practical expertise in avoiding pitfalls when using powder XRD, *i.e.* factors that result in mistakes and discrepancies such as those associated with sample preparation; texture and preferred orientation of the crystallites; apparatus effects; position, thickness and roughness of the sample; and asymmetry.

All participants expressed an interest in participating in future workshops on powder XRD devoted to detailed and complex approaches that give valuable information for a wide range of materials. This workshop appeared to be a good model for collaboration between the Institutes of the BAS, Bulgarian universities and commercial companies.

International Autumn School on Fundamental and Electron Crystallography (IASFEC)

This School took place in the BAS Hotel, situated at the BAS Campus I in Sofia, from 8 to 13 October 2017. The main purpose of the School was to introduce the theoretical background of fundamental and

electron crystallography to the participants and trainees, and to provide the young crystallographers with the opportunity to present their research results and exchange new ideas.

The School started with a half-day course, 'Introduction to Matrix Algebra', provided by Mois Aroyo (University of Basque Country, Bilbao, Spain). The topics of the School programme were divided into two parts. The first included 14 lectures dedicated to fundamentals of crystallography, presented by Massimo Nespolo (University of Lorraine, Nancy, France) and Mois Aroyo, both consultants and former chairs of the IUCr Commission on Mathematical and Theoretical Crystallography. The second part was composed of 17 lectures that illustrated the principles of electron crystallography, presented mainly by Joke Hadermann (University of Antwerp, Belgium). The main subjects were indexing of an electron diffraction (ED) pattern; calculation/simulation of a selected area (SA) ED pattern for a given compound (from cell parameters and zone axis); reconstruction of the unit cell from an SAED along different zone axes; connection of the symmetry in real space to that of the ED pattern; converged-beam ED; superlattices (subcells) and sublattices (supercells); and the determination of point groups and space groups from ED patterns.



Participants at IASFEC 2017.

The 48 people who attended the school came from 11 countries and included 33 participants, the 3 invited speakers and the 12 members of the local organizing committee. Among the 33 participants (19 from Bulgaria), 23 were young scientists (PhDs, postdocs and junior researchers). Nine of them had been fully or partially supported by travel and subsistence grants.

Short Course Workshop: Intensive Practical Course on Powder X-ray Diffraction

In the period 5-8 November 2017, a group from the Geological Survey of the Republic of Kosovo and the University of Mitrovica 'Isa Boletini' in Kosovska, Mitrovica, visited IGIC-BAS and IMC-BAS. The Kosovan

guests participated in this short course workshop, which was organized by the BCS and the two Bulgarian institutes.



The guests from the Republic of Kosovo in the XRD lab of the IGIC-BAS.

The lectures presented basic knowledge of the crystallographic description of solid substances, the features of X-ray radiation and its use in the analysis of powder materials. The exercises were devoted to qualitative and quantitative phase analyses of geological and mineralogical samples. The colleagues from Kosovo showed interest in collaborating with the BAS institutes to obtain help and support in working with different apparatus for the investigation of materials, education in the framework of the PhD programmes in BAS, as well as participation in future scientific events in Bulgaria.

This short course workshop is a good example of collaboration between the countries in the Balkan region in action.

For forthcoming meetings in Bulgaria, see <https://www.iucr.org/world/bg>.

OUTREACH

Winners of the 2017 IUCr Crystal Growing Competition



IES Heliópolis, Sevilla (Spain): bronze medal winners in the 15-18 year-old category.

Continuing the success of the crystal growing competition that launched during IYCr2014, we are delighted to announce the winners of the 2017 IUCr Crystal Growing Competition.

Schoolchildren were invited to convey their experiences of growing crystals through a video. The entries were judged on their creativity, aesthetic value, description of the working plan and experimental work, clarity of explanation, scientific background and safety by an international panel. The winners, who will receive a certificate and medal, are as follows:

Category: 15-18 - GOLD: IES Valle del Andarax, Canjáyar (Spain); SILVER: Wellspring International Bilingual School, Hanoi (Vietnam); BRONZE: IES Heliópolis, Sevilla (Spain)

Category: 11-15 - GOLD: Bedok South Secondary School (Singapore); SILVER: Wellspring International Bilingual School, Hanoi (Vietnam); BRONZE: Sint-Barbaracollege, Gent (Belgium)

Category: Under 11 - GOLD: Escuela San José de Calasanz, San Juan (Argentina); SILVER: Escuela No. 65, Treinta y Tres (Uruguay); BRONZE: Escuela No. 65, Treinta y Tres (Uruguay)

and the winning videos can be watched [here](#).

The [2018 IUCr Crystal Growing Competition](#) is now open. The deadline for submission of videos is 18 November 2018. Please note that videos submitted to local competitions during 2018 may also be submitted to the IUCr competition.

OUTREACH

Teaching crystallization in secondary schools in Kenya

Juan Manuel García-Ruiz



The European Research Council project Prometheus aims to explore the role of mineral self-assembly in the early Earth and its plausible role in primitive life detection and the origin of life. Within the project, we have to travel to remote places in search of silica-rich alkaline waters and other extreme geochemical environments. We like to explain to the people of the regions we visit what we are looking for and why. When possible, we also like to deliver popular lectures for high-school students and teachers on fundamental aspects of crystallization and its application to everyday life.

One of the places we are investigating is the Eastern branch of the East African Rift Valley, the so-called Soda Lakes. In March 2016, we delivered a four-hour course for teachers, students and authorities in Limuru, north of Nairobi. I also delivered a lecture in the Louis Leakey auditorium at the National Museum of Kenya.

In March 2018, I gave lectures in two very different Kenyan secondary schools. The first was a private school called Nova Academy near Nairobi, the second a public school in a remote site called Magadi, in the land of the Masai people.



This sample of huge crystals of trona was highly appreciated by the students.

My experience with the Kenyan school system is that primary and secondary education is a priority issue for this country. For all schools in the country, from those in Nairobi or Mombasa to those in the remote parts of the African savannah, electricity is compulsory, and in many of them, students have access to tablet computers. Another feature that is obvious is that the quality of teachers of primary and secondary education is very high and most of them show an enviable degree of professional commitment.

Another characteristic of Kenyan schools is the high degree of interest shown by the majority of students. In both private and public schools, students show an enormous disposition to learning and a clear determination. It is striking that beyond the high-quality average, there are a significant number of brilliant students in Kenya. This country thus ensures a pool of leaders for the future. At the Nova Academy, students were the absolute protagonists. They prepared themselves a lovely introduction to the talk with information they collected from the web. Impressive!



Tata Chemicals Magadi, previously Magadi Soda Company, has been mining trona, $\text{Na}_2\text{CO}_3 \cdot \text{NaHCO}_3 \cdot 2\text{H}_2\text{O}$, from Lake Magadi since 1911. We are collaborating with the company to develop a 'crystallization kit' to trigger the teaching of crystallization in the schools of Kenya and throughout Africa. The University of Nairobi and Patricia Gitari from D-Orbital Limited are involved in this project.

I would like to thank the CSIC Outreach Department and the IUCr for providing materials for the students and teachers.

Juan Manuel García-Ruiz is currently with CSIC and University of Granada, Spain.

This is a condensed report. See the full version [here](#).

OUTREACH

LACA President Diego Lamas talks crystals on Argentinian TV



Diego Lamas, President of the [Latin American Crystallographic Association](#), recently participated in the Argentinian TV show '*todo tiene un porqué*' ('Everything has a reason') aired by the TV Pública Argentina channel. On this occasion, the program was dedicated to explaining what a geode is and, in that context, Diego was invited to explain how crystals are formed and demonstrate simple experiments that can be performed at home or school. For example, he explained how to make beautiful crystalline sugar sticks and how to imitate a geode by growing crystals in an eggshell. He also explained the main topics studied in Crystallography and commented on some of the work presented in the [Argentinian Crystal Growing Competition for Secondary Schools](#) and in the [IUCr Crystal Growing Competition for schoolchildren](#).

Here is a [link](#) to the program, in Spanish, on the Argentinian TV site.



Diego Lamas (center) explains how to obtain sugar polycrystals from a seed crystal.

"Todo tiene un porqué" is a cultural, educational and scientific magazine of federal character; its purpose is to offer the audience solid and attractive content that can teach while entertaining. The content presented in the program raises questions that seek answers in different disciplines (physics, chemistry, psychology, sociology, philosophy, biology, anthropology, etc.) and is supported by scientific advisors who analyze and check the rigor of the information, which is presented in a dynamic and varied style. With the participation of scientists, researchers and other invited experts, this TV show aims to stimulate in viewers the desire to know more and even generate interests that could become future vocations.

MEETING REPORT (IUCR SUPPORTED)

Workshop on Modern Trends in Mathematical Crystallography

Ma. Louise Antonette N. De Las Peñas



In recent years, the area of mathematical crystallography has grown beyond the traditional study of the fundamental properties of symmetry and periodicity of crystals. This expanded horizon was the subject of the workshop 'Modern Trends in Mathematical Crystallography' (MathCryst Manila 2017), held in the Ateneo de Manila University in Quezon City, Philippines, from 20 to 24 May 2017, which introduced participants to current topics and new directions in mathematical crystallography and its applications. New trends in group and graph theory, as well as topological aspects of mathematical crystallography, were focal points. In this second mathematical crystallography workshop held in the country (the first one dates back to November 2011), there were eight invited speakers, experts in their respective fields, who gave talks on topics ranging from discrete models of crystals, periodic to aperiodic, to highly ordered structures. The expected outcomes of the workshop for the participants included exposure to research opportunities in mathematical crystallography, heightened awareness of the relevance of crystallography in their research, and starting or continuing collaborations between researchers.

The workshop began with a brief opening programme, where Ateneo de Manila University officials welcomed the speakers and participants. Ma. Louise Antonette De Las Peñas, Local Organizing Committee Chair, gave the participants an overview of how mathematical crystallography started in the Philippines. The workshop proper followed, starting with a lecture from Jean-Guillaume Eon (Federal University, Rio de Janeiro, Brazil) about the *Topology of Crystal Structures: Applications of Graph Theory* and followed by a lecture on *Domain Structures* by Massimo Nespolo (University of Lorraine, France). On

the second day of the workshop, Egon Schulte (Northeastern University, Boston, MA, USA) and Stephen Hyde (Australian National University, Canberra, Australia) lectured, respectively, on *Polyhedra, Complexes, Nets, and Symmetry* and *Two Dimensional Crystallography via Orbifolds*. On the third day, participants explored the *Bilbao Crystallographic Server: Mathematical Crystallography Tools in Material Studies* through a workshop conducted by Mois Aroyo (University of the Basque Country, Bilbao, Spain). Dirk Frettlöh (Bielefeld University, Germany) gave two lectures, *Quasicrystals and Symmetry* on the third day, and *Average Lattices for Quasicrystals* on the fourth day. Shigeki Akiyama (Tsukuba University, Japan) gave a lecture on *Beta Expansions and Self-Affine Tilings*, also on the fourth day. Finally, on the fifth day, Marjorie Senechal (Smith College, Northampton, MA, USA) gave a lecture on *Icosahedral Snowflakes*.



Local Organizing Committee with speakers.

MathCryst Manila 2017 had 65 participants, including 14 members of the Local Organizing Committee. 19 participants presented posters during a poster session on the third day of the workshop, showcasing their research related to mathematical crystallography. The organizers set up tea and lunch breaks to give time for socialization and relaxation, as well as opportunities for participants to have discussions among themselves and with the speakers about mathematics and crystallography. Very notable was the fact that the students were very eager and excited to interact with the speakers and ask questions. For most of the students, this was their first chance to attend an international workshop and to learn about mathematical crystallography.

During the final programme held on the last day of the workshop, gifts of appreciation were given to the speakers, and certificates of attendance distributed to the participants by the Local Organizing Committee. A couple of participants were asked to speak about their experiences during the workshop. Gwendolyn Tadeo, a graduate student of the Ateneo de Manila University, spoke on behalf of the other students in attendance, and summarized her experience as follows: 'This has been a venue for me, for us, to learn more about the area of crystallography, how really beautiful it is, and opens the possibility of exploring more of its beauty with the help of mathematics. With all the talks that we had from our

speakers, I would use the words *overwhelming* and *profound* to describe the experience of being able to listen, comprehend and digest everything that has transpired the past five days. I'll say after this workshop, I'm already trying to consider a research area related to tilings or crystallography. It was such a great experience to have attended this workshop, and this experience has made me realize again and again, that as long as there are questions to be asked, and answers to be found, mathematicians never stop'.



IUCr Young Scientist Awardees.

MathCryst Manila 2017 would not have been a success if it were not for the speakers' generosity and commitment, the hardworking members of the Local Organizing Committee from the Department of Mathematics, Ateneo de Manila University, and the help and sponsorship of the South East Asian Mathematical Society (SEAMS), the Mathematical Society of the Philippines (MSP), and the Ateneo de Manila University. Special mention goes to the IUCr and its Commission on Mathematical and Theoretical Crystallography for the organizational support, travel support for visiting professors and young scientists to attend the workshop, and above all for providing the opportunity to have a second mathematical crystallography workshop in the Philippines.

We hope that with this workshop, more fruitful collaborations will spring forward, and that current research partnerships will be further strengthened. We certainly are looking forward to a third mathematical crystallography workshop in the Philippines in the near future!

MEETING REPORT

25th Slovenian-Croatian Crystallographic Meeting



Plenary lecturers (l-r): H. Puschmann, J.K. Cockcroft, E. Boldyreva, D. Stalke and K. Molčanov (missing M. Marinšek).

The 25th Slovenian-Croatian Crystallographic Meeting was held in June 2017 in the city of Ljubljana, Slovenia, in the newly built Faculty of Chemistry and Chemical Technology. There were 79 registered participants from Austria, Germany, India, Russian Federation, South Africa, UK, Croatia and Slovenia. Five plenary lectures were presented: 'High-pressure studies of organic and coordination compounds' (Elena Boldyreva, Novosibirsk, Russia), 'More than 100 years of Lewis diagrams - still valid in the light of charge density?' (Dietmar Stalke, Göttingen, Germany), 'Powder diffraction: an essential complementary tool for those skilled in the art but one with pitfalls for the unwary' (Jeremy Karl Cockcroft, London, UK), 'Stacking of planar conjugated rings - beyond aromatics' (Krešimir Molčanov, Zagreb, Croatia) and 'Microstructure evolution in cermet anodes for solid oxide fuel cells' (Marjan Marinšek, Ljubljana, Slovenia). To enrich the programme of the meeting, an *Olex2* workshop was also organized (Horst Puschmann, OlexSys and Durham University, UK).

One of the advantages of the Slovenian-Croatian Meetings is that all participants give an oral presentation, which gives young scientists the opportunity to present their work in a friendly but professional atmosphere. 59 short oral presentations addressed contemporary topics in crystallography: structure determination of organic, inorganic and coordination compounds; crystal architecture and design; phase transitions; solid solutions; structure-property relationships; synergy of diffraction and complementary techniques; and history.

The meeting was organized jointly by the Faculty of Chemistry and Chemical Technology, University of Ljubljana, and the Croatian Crystallographic Association under the auspices of the University of Ljubljana, and promoted by the Slovenian Chemical Society. There was no registration fee. Therefore we thank the sponsors, donors and advertisers: European Crystallographic Association, Renacon, Rigaku, Bruker, MiTeGen, Crystal Impact, Stoe, Dectris, Mettler Toledo, Aparatura, Lek-Sandoz, Laboratorij-um and Scan.

More information about the meeting can be found [here](#).

MEETING REPORT

20th Heart of Europe Bio-Crystallography Meeting

Milton T. Stubbs



Any meeting that has reached its 20th anniversary must have found a winning formula, and Matthias Bochtler and Marcin Nowotny of the International Institute of Molecular and Cell Biology in Warsaw, Poland, applied this formula in exemplary fashion within the fairytale Wojanów Palace at the foot of the Karkonosze Mountains in southwestern Poland from 28 to 30 September 2017.

HEC20 was attended by structural biologists from 22 laboratories in central Europe (Austria, the Czech Republic, Germany and Poland), with PhD students and young postdocs presenting current topics of their research. The quality of their talks was high, making it hard for the HEC Prize Committee to reach its decision. After much deliberation, Ronja Janke (FU Berlin, Germany) was awarded a copy of the IUCr-sponsored *State of the art of Macromolecular Crystallization* for her presentation *Insights into the catalytic mechanism of CotB2*. The HEC lecture, presented each year by a prominent scientist outside the HEC community, was delivered by Tim Clausen (IMP Vienna, Austria). His talk *The phospho-kiss of death: revealing a specific phospho-signal that serves as degradation tag* was truly inspirational, demonstrating how structural studies can open up whole new areas of biology.



Ronja Janke (right) receives her prize for the best student lecture from Pavlína Řezáčová.

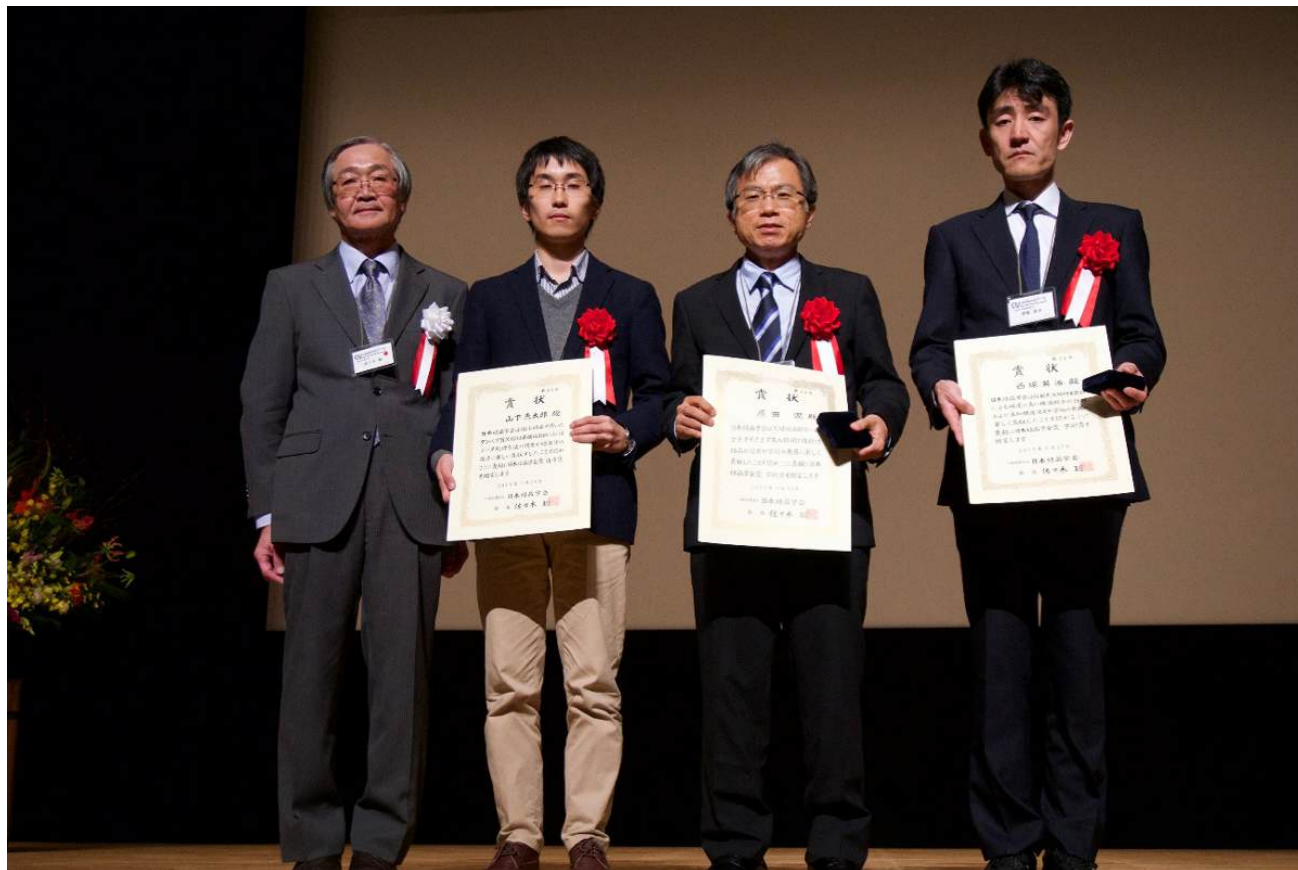
Interspersal of the talks with short company-sponsored presentations served to introduce new technologies to the participants, and the hearty Polish food and drink fostered a warm atmosphere for both formal and informal discussion. The afternoon visit to Karpacz provided something for everyone, with a tour of the Vang stave church for those culturally inclined, a walk up to the Pielgrzymy rocks for the sprightlier, and a hike to the top of the Śnieżka for the sprightliest.

Matthias, Marcin and Małgorzata (Gosia) Figiel are to be thanked for the excellent organisation of HEC20. [HEC21](#) will take place between 20 and 22 September 2018 in the German medieval town of Quedlinburg in the Harz Mountains.

MEETING REPORT

2017 Annual Meeting of the Crystallographic Society of Japan

Takashi Ohhara



Recipients of the CrSJ17 Awards with the President of CrSJ. l-r: Sasaki (President), Yamashita, Harada and Nishibori.

The 2017 annual meeting and the general assembly of CrSJ (CrSJ2017) was held from 23 to 24 November at the JMS Aster Plaza in Hiroshima, Japan; about 300 crystallographers participated. The meeting featured 47 oral and 116 poster presentations covering all aspects of crystallography, three award lectures, three microsymposia, a special lecture promoting gender equality, two luncheon seminars and an industrial exhibition involving 13 companies/organizations. The microsymposia were titled 'Innovation in materials science invoked by crystallography beyond the Bragg peaks', 'Fascinating crystalline organic, coordination and inorganic compounds displaying various structures and functions' and 'Innovations in nucleic acid structural biology using synchrotron X-rays'; a total of 13 invited talks were given.

At the CrSJ Awards Ceremony, the Research Award was given to Eiji Nishibori (Tsukuba University) for his research 'Synchrotron X-ray powder diffraction studies of accurate structure-factor measurements and *ab initio* structure determination' and Jun Harada (Hokkaido University) for his research 'Dynamics of molecules in crystals: X-ray crystallographic analysis and development of functional materials'. The Young Crystallographer Award went to K. Yamashita (RIKEN) for his research 'Development of an X-ray data processing system for protein micro-crystals'.

Four young scientists were honored with Poster Awards: K. Hibino (Tokyo Institute of Technology), H. Kiyooka (Hyogo Prefecture University), T. Nakane (University of Tokyo) and K. Takaba (Kyoto University).



The Poster Awardees and the President of CrSJ. l-r: Sasaki (President), Takaba, Nakane, Kiyooka and Hibino.

The Young Crystallographers' Meeting 2017, a satellite meeting of CrSJ2017, was held on 22 November at the Hiroshima Synchrotron Radiation Center (HiSOR), Hiroshima University; 30 researchers/students participated. This meeting is held every year to give young researchers and graduate students the opportunity to communicate and network with each other, especially beyond the barriers between physics, chemistry and biology, in an informal environment. On this occasion, lectures were given by K. Matsuo (Hiroshima University), S. Shimono (Osaka Prefecture University) and T. Jindo (Yokohama National University), which were followed by a tour of HiSOR as a special event of the meeting, and a banquet.

A full program of the meeting can be viewed [here](#). The chair of the organization committee was Y. Kuroiwa (Hiroshima University) and the program committee was chaired by C. Moriyoshi (Hiroshima University).

The [2018 annual meeting](#) will be held from 10 to 11 November 2018 at Ookayama campus of Tokyo Institute of Technology. The chair of the organization committee is M. Yashima (Tokyo Institute of Technology) and the program committee is chaired by H. Uekusa (Tokyo Institute of Technology).

MEETING REPORT (IUCR SUPPORTED)

1st LACA School: Small-Molecule Crystallography

Leopoldo Suescun Natalia Alvarez Guzmán Peinado



1st LACA School: Small Molecule Crystallography

- Primera Escuela de la LACA: Cristalografía de Moléculas Pequeñas -

19-25 de febrero de 2018 - Facultad de Química - Universidad de la República
Montevideo - Uruguay



The first Latin American Crystallographic Association school devoted to small-molecule crystallography (1LACASSMC, <http://lacassmc.fq.edu.uy/>) was held from 19 to 25 February 2018 at the Facultad de Química, Universidad de la República, Montevideo, Uruguay. Profiting from the momentum gained from the organization of two IUCr/UNESCO OpenLabs in 2014 and 2016, the core of the organization and lecturers from these events (Leopoldo Suescun and Natalia Alvarez from Uruguay, Javier Ellena and Hamilton B. Napolitano from Brazil, and Bruce Noll from USA) was spiced-up for this first official LACA school, which is actually a continuation of a long tradition of regional education in crystallography. The addition of Florencia Di Salvo (Argentina), Vojtech Jancik (Mexico), Silvina Pagola (USA) and Tony Linden (Switzerland) to the cohort of lecturers provided the school with the best of the region's small-molecule crystallographers and lecturers, plus an international flavor.

The Local Organizing Committee (Leopoldo Suescun, Natalia Alvarez and Guzmán Peinado from Facultad de Química) obtained financial support from the IUCr, Bruker AXS, Agencia Nacional de Investigación e Innovación, D2C2-Ministerio de Educación y Cultura, ASM SRL (Bruker representative in Uruguay), FUNDAQUIM and PEDECIBA (Uruguay) and the Cambridge Crystallographic Data Centre to grant travel and local expenses support for students from all over Latin America. The event brought together 39 participants (professors, postdocs, PhD, MSc and undergraduate students) from Argentina (6), Bolivia (1), Brazil (8), Chile (4), Colombia (2), Costa Rica (1), Guatemala (1), México (2), Panamá (1), Paraguay (1) and Uruguay (11). They all had the chance to learn the fundamentals of crystallography and the

application of single-crystal and powder X-ray diffraction to the study of small-molecule structure. In addition, participants experienced all the processes of single-crystal X-ray diffraction, from crystal selection and mounting to CIF preparation, with practice samples and data. The practical aspects of the school centered on the Bruker D8 Venture diffractometer, installed in 2014, and APEX3 software. The students were provided with temporary licenses for the software and the Cambridge Structural Database to complete their structural analysis and learn about databases. Additionally, over a dozen very excited participants brought single crystals and were able to select and mount them, collect their own data, and perform the structure determination and refinement of the structures themselves with the assistance of tutors, lecturers and fellow participants.

The school program included 20 hours of lectures and 5 hours of practical sessions on the fundamentals of crystallography taught in Spanish by Professors Di Salvo (INQUIMAE, Universidad de Buenos Aires, Argentina), Ellena (Instituto de Física de São Carlos, Universidade de São Paulo, Brazil), Jancik (Departamento de Química, UNAM, Toluca, Mexico), Pagola (Hampton University, VA, USA) and Suescun (Facultad de Química, Universidad de la República, Montevideo, Uruguay). Moreover, 6 hours were taught in Portuguese by Professor Napolitano (Universidade Estadual de Goiás, Brazil) and 14 hours in English by Professor Linden (Department of Chemistry, University of Zurich, Switzerland) and Bruce Noll (Bruker AXS, Madison, WI, USA). During the practical sessions and data handling sessions all lecturers and the tutor (N. Alvarez) were available for discussion. Starting on Wednesday, the participants who had brought crystals had the opportunity to collect data with Bruce Noll.

The intense program included a social dinner held on Wednesday and a free afternoon that allowed the majority of the participants to catch up with the topics and work on their own problems (in addition to sightseeing in Montevideo in the evening).



Top row, l-r: Professor Linden (Switzerland) presenting the opening lecture; participants at the opening lecture; Professor Jancik (Mexico) lecturing on the use of *SHELX* to solve disordered structures. Bottom row, l-r: social dinner; Miguel Martínez (Paraguay) and João de Araújo (Brazil) talk about crystals while Bruce Noll (USA) in the background checks a data collection run; Maia Mombrú (Uruguay) presents the results of her structure determination and refinement of a salicylic acid crystal grown by high school students who won the 2017 national crystal growing competition (see <http://www.cncc.fq.edu.uy/>).

On Saturday afternoon, 5 hours were dedicated to finishing the participants' problems, such as refining disordered and twinned crystals and even structures with powder diffraction data using *WinPSSP* software [Pagola, Polymeros & Kourkouvelis (2017), *J. Appl. Cryst.* **50**, 293-303]. Sunday morning was devoted to student presentations given by 8 of the participants who solved their own problems or available data, and an exam taken by 23 participants who will receive academic credit for their participation in 1LACASSMC, completing the total of 55 hours.

An anonymous evaluation form was provided for the students to give their own opinions on different aspects of the school. Except for the unanimous feeling that the course was very intense, the large majority of comments were positive and some helpful remarks were given that will help organize future schools of this kind in Latin America. A detailed report of the opinions of participants given in the evaluation form can be downloaded from our official website, <http://lacassmc.fq.edu.uy/>.

MEETING REPORT (IUCR SUPPORTED)

2018 Powder Diffraction and Rietveld Refinement School

Ivana Radosavljevic Evans



The 2018 Powder Diffraction and Rietveld Refinement School (Durham, UK; 8-12 April 2018) combined lectures, small-group tutorials and hands-on computer practical sessions. The lectures introduced the basic concepts of crystallography, powder diffraction and Rietveld refinement. Both by-hand and computer-based tutorials were problem-based learning oriented. For each hour of lectures there was at least an hour scheduled for small-group problems that were led by lecturers and tutors who helped reinforce the concepts. The remaining ~50% of the course was spent with students working through computer practicals at their own pace. There were over 70 computer-based problems and exercises available on a range of different topics, from basic peak fitting and powder-pattern indexing to advanced state-of-the-art diffraction data analysis methodologies, including parametric/surface fitting and distortion mode analysis. The structure of the course is such that everyone was introduced to and given some training in all aspects of crystallography (and data collection using different types of sources on different types of samples), but ultimately had the flexibility to spend more time learning and practising the material most relevant to their own research areas.

The international dimension

Funding received from the IUCr supported the attendance of seven early-career scientists: Anne Whitworth (Monash University, Australia), Mauro Coduri (ESRF, France), Katarzyna Kosyl (Institute of Physics, Polish Academy of Sciences, Poland), Evgeny Filatov Nikolaev (Inorganic Chemistry Institute,

Russia), Eleonora Isotta (Trento University, Italy), Joaquin Grassi (Republica University, Uruguay) and Van Huan Doan (Hanoi University of Mining and Geology, Vietnam). In addition, we managed to secure additional support from industry and Durham University, which helped more international students attend the School. In fact, overseas participants constituted 31 out of 64 students (48%); they came from 20 different foreign countries (in Europe, North America, South America, Asia and Australia): France, Vietnam, Russia, Germany, Switzerland, Romania, Uruguay, Denmark, Korea, Poland, India, Mexico, Australia, Sweden, Canada, Italy, Slovenia, Norway, USA and Japan. In addition, 10 of the remaining participants were overseas students pursuing their PhDs at UK institutions, some of whom are likely to return to their home countries and disseminate the knowledge acquired here. This brings the total international participation at Durham PDRR 2018 to 41 out of 64 participants (64%), and reflects the true scale of the international character of the School.

We believe that the School was a success and addressed a need for key training in the UK and internationally.

MEETING REPORT

1st Intensive School in Physical Crystallography: From Phonons to Phase Transitions

Mark S. Senn



The Physical Crystallography Group (PCG) of the British Crystallographic Association was pleased to be able to offer its first residential school in physical crystallography in Abingdon, Oxfordshire, UK, from 18 to 21 June 2018. Planning for the School started back in January 2017 when the organising committee consisting of myself, Mike Glazer, John Claridge and Nick Funnell undertook the initial task of shortlisting topics for the school. We quickly homed in on the key material that we felt would be most beneficial to the community, from which everything else followed naturally. We decided for the first run of the PCG School we would focus on phase transitions, since the study of this topic is what unites all physical crystallographers. We were keen to include topics such as phonons and Landau theory in this that are not so commonly taught as part of postgraduate courses. We were delighted that Martin Dove and Michael Carpenter were willing to take on these topics and keen to be involved in this new project. The course was structured to follow the path of a soft-mode phase transition, with the final line-up of Mike Glazer for a review of symmetry and reciprocal space, Martin Dove for phonons, myself for irreducible representation analysis, Michael Carpenter for Landau theory, and John Claridge for incommensurate phase transitions. Our ambitious plan was now to fit this program into a 3.5-day intensive residential school. We were very fortunate in receiving substantial sponsorship from the ISIS Neutron and Muon Source, as well as contributions from Diamond Light Source and the Institute of Physics. This meant that we could hold the event with a substantially reduced residential registration fee of £240, whilst still being

able to make use of STFC's unique Cosener's House venue situated in the picturesque town of Abingdon on Thames. Special thanks go to Nick Funnell here, who took on the bulk of the local organising leading to a seamlessly run school.

On midday on 18 June 2018, after months of planning, we were finally ready to welcome the 40 school participants, many who had travelled from afar. Registration for the School had far exceeded our expectation, making it a tough process shortlisting the candidates for the school. The final list of course participants included PhDs, post docs and early career academics from the Netherlands (5), Germany (2), USA (1), South Korea (1), Australia (1), Spain (1), France (1) and Republic of Ireland (1), with the rest coming from all around the UK.

Mike Glazer opened the school with a review of point-group and space-group symmetry for his first lecture, before developing the idea of reciprocal space, the appreciation of which would be crucial for the students' understanding in the following lectures. After a coffee break during which the sunshine and beautiful surroundings of Cosener's House could be enjoyed, it was back to work. Mike had prepared a lovely practical exercise helping the students gain familiarity in identifying symmetry elements, and helping them appreciate how *International Tables of Crystallography* Volume A is constructed.

As we had promised the students, the school would be intensive, which meant that after a three-course meal served back in the main building of Cosener's House, we returned to work. This time it was a poster session giving students the chance to present their work to each other, and it was also a great chance for the lecturers to get an idea of the research areas that the students were working in. I particularly enjoyed this session and was impressed by both the breadth and diversity of research topics covered by the course participants, and by how many students stayed on well past the point at which the free drinks ran out!

On Tuesday morning, fuelled by a full English breakfast, Martin Dove took the reins. He started out with a nice historical introduction to the field of lattice dynamics, before diving into the detail behind phonons and normal modes. The link between the theory of soft-phonon-mode phase transitions and Landau was beautifully made, and Martin finished his lectures with some nice examples of the effect of rigid-unit-mode motion on phonon dispersion and diffuse scattering. This *tour de force*, followed by a practical session using *GULP*, took the students through from 9am to 5pm - interspersed with plenty of breaks of course!

I was up next. I was a little nervous, not least as I had scheduled my lectures for the shift before and after dinner in what I appreciate was already a very long day for the students. My goal was to describe the language through which symmetry-breaking events can be classified according to irreducible representations. I was keen for the students to grasp that this symmetry breaking could be instantaneous, such as the dynamic fluctuations induced by phonons, or that it could be related to the order parameters describing the long-range ordering occurring at phase transitions. My tutorial session, which saw the students return fresh-faced on the Wednesday morning, sought to reinforce these concepts through several exercises, using *ISODISTORT* to analyse phase transitions and degeneracy in phonon-dispersion curves.

It was then over to Michael Carpenter who gave a very nice illustration of how the coupling between primary order parameters and strain can be used to study the nature of phase transitions, within the framework of Landau theory. As well as providing practice at performing this kind of analysis, the tutorial sessions explored how, once the Landau potential has been constructed, a host of other thermodynamic quantities can be derived and interrogated. It was particularly impressive to see the enthusiasm and stamina of the students throughout these sessions, who, even come the evening, were still working hard at problems and asking questions.

We felt it was also important for the students to appreciate how experimental measurements probing lattice dynamics can be made and interpreted, and in this respect we were very lucky to have two guest speakers on Wednesday afternoon from the ISIS Neutron and Muon Source. David Voneshen and Matthias

Gutmann talked about their research interests around inelastic neutron scattering and diffuse scattering, providing an extra dimension to the school's curriculum. Even after such an action-packed Wednesday, I was pleased to see that a substantial number of students found the energy to soak up the last rays of sunshine by the river Thames, over a drink or two at the Nags Head Pub.

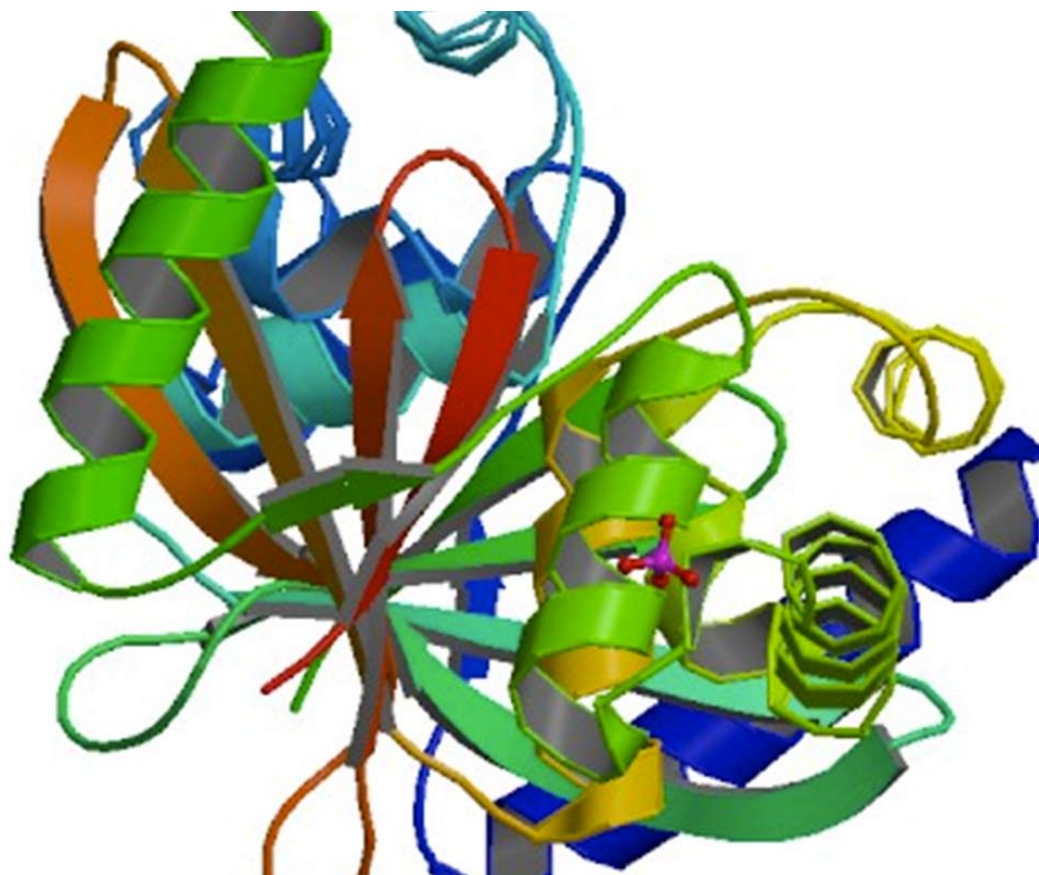
On Thursday morning it was over to John Claridge who gave an introduction to the superspace formalism and incommensurate crystallography, before diving into many intriguing examples of incommensurate phase transitions in functional materials. These ranged from site-occupancy modulation in thermoelectrics, to lone-pair and incommensurate tilt ordering in ferroelectric materials. For the final tutorial session, the students were let loose on refining incommensurately modulated structures in the program *Jana2006*.

As lecturers, we were very impressed by the calibre of the students and their enthusiasm, which was sustained up until the final session. For me, this is what really made the school so special. We hope to return for the 2nd PCG School in Physical Crystallography in 2020, but in the meantime the lecture material is available [here](#) for all to enjoy.

ADVERTISING FEATURE

The MORPHEUS III protein crystallization screen: at the frontier of drug discovery

Fabrice GorrecGiovanna Zinzalla



Q&A with Fabrice Gorrec, inventor of the screen

Dr Gorrec has participated in the development of innovative technologies applied to protein crystallization for over 15 years, including microplates (e.g. TOPAZ), liquid handlers (e.g. dragonfly) and initial screens (e.g. MORPHEUS). Since 2007, Fabrice has been responsible for the crystallization facility at the Medical Research Council Laboratory of Molecular Biology (MRC-LMB, Cambridge, UK) where he invented and developed the 96-condition MORPHEUS protein crystallization screens. The corresponding approach to formulation has recently been presented as part of the [IUCr's webinar series](#).

Why are you developing more crystallization screens?

The novel samples required to study biological mechanisms at the atomic level are increasingly challenging to produce and crystallize. Besides, there are additional difficulties in making X-ray crystallography amenable to the discovery of drug compounds (Müller, 2017). Subsequently, innovations that enhance the yield of useful crystals are urgently required. The original [MORPHEUS](#) (Gorrec, 2009) has proven to be a very efficient protein crystallization screen in the long term for a broad variety of protein samples, and the first follow-up, [MORPHEUS II](#) (Gorrec, 2015), has started to have an impact for many research groups (Fig. 1). To date, MORPHEUS conditions have been mentioned 317 times in the (vastly unreported) field 'crystal growth procedures' in the Protein Data Bank (PDB).

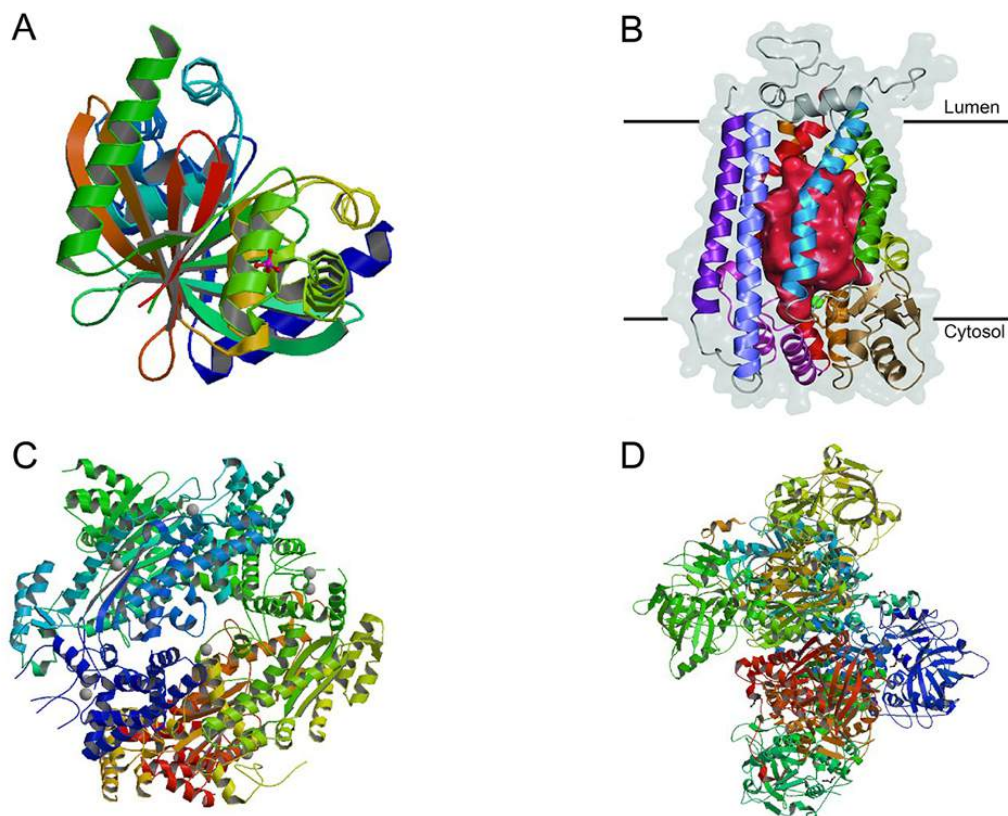


Figure 1. Examples of crystal structures solved after using either MORPHEUS I or II. A, Human Ovarian Tumor Deubiquitinase (OTU DUB1) (Mevisen *et al.*, 2013; PDB ID: 4BOP). The 16 human OTU DUBs cleave distinct sets of ubiquitin chain types. B, Integral Membrane Protein CAAX Protease Ste24p (from Pryor *et al.*, "Structure of the Integral Membrane Protein CAAX Protease Ste24p", *Science*, **339**, 2013, reprinted with permission from AAAS), a zinc metalloprotease involved in two proteolytic steps for the maturation of yeast mating pheromone α -factor. C, Cmr2 from *Pyrococcus furiosus* (Benda *et al.*, 2014; PDB ID: 4W8Y). The Cmr complex is an RNA-guided endonuclease that cleaves foreign RNA targets as part of the CRISPR prokaryotic defense system. D, *Klebsiella pneumoniae* 3,4-dihydroxybenzoic acid decarboxylase (AroY), an enzyme involved in *para*-carboxylation of catechols (Payer *et al.*, 2017; PDB ID: 5O3M).

What about MORPHEUS III?

The main ideas behind the formulation of the new screen were the same as those for MORPHEUS I and II, which are essentially:

- Increasing the chances of crystal nucleation and growth by integrating mixes of additives that can act as stabilizers, cross-linkers, *etc.* (McPherson & Cudney, 2006).
- Providing systematic approaches to selecting the reagents and formulating the screen, including the integration of ligands found in the PDB.
- Enhancing pragmatic ways to facilitate the steps towards structure solution, notably with cryoprotected conditions.

The novelty in MORPHEUS III is the integration of small drug-like compounds as additives (average MW = 248 Da). To some extent, the approach can be compared to fragment-based lead discovery (Blundell, 2017). In this perspective, MORPHEUS III is at the frontier of drug discovery. The primary aim, however, is still to obtain useful crystals from a broad variety of novel samples.

The final formulation of the new 96-condition crystallization screen integrates 44 compounds overall, divided into 8 mixes of additives. Each mix of additive is combined with 4 cryoprotected precipitant mixes and 3 buffer systems to form a three-dimensional grid (see Fig. 2). The set of single compounds has been used to formulate an additive screen called [HIPPOCRATES](#). It will be interesting to search the

PDB for MORPHEUS III compounds in the future and see if they are more represented because they were integrated into commercially available screening kits.

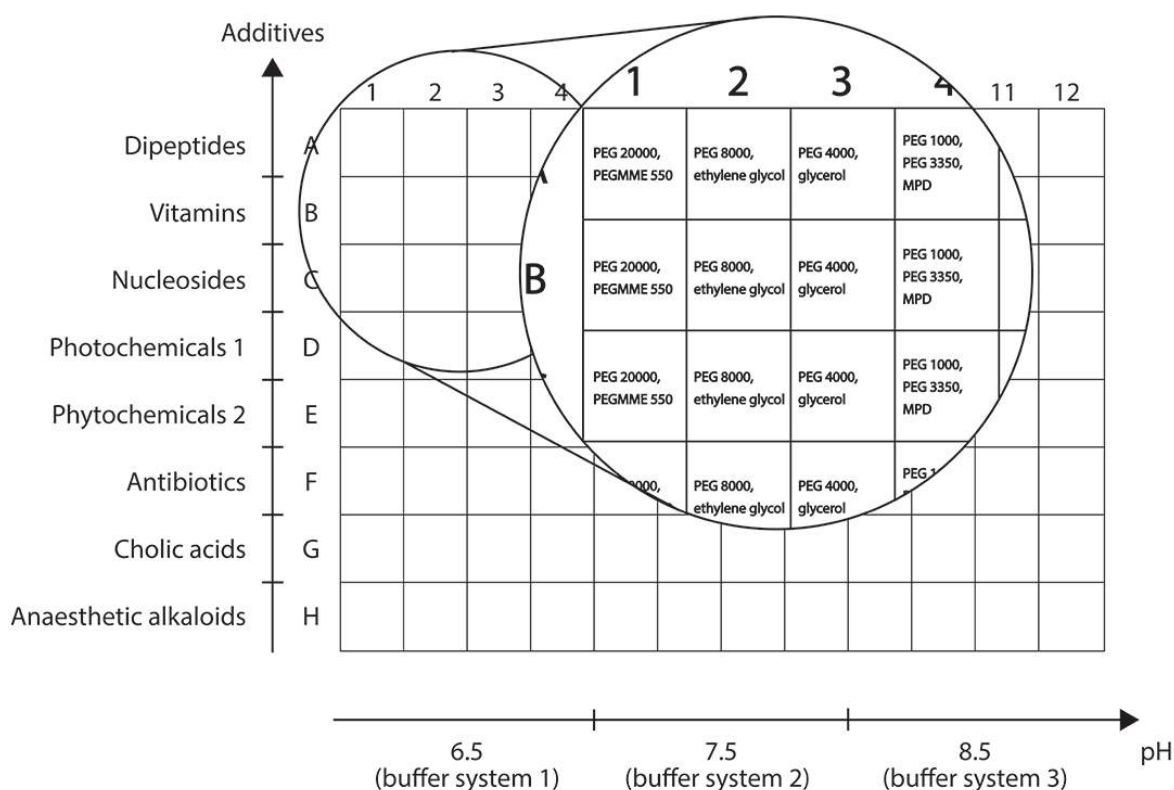


Figure 2. MORPHEUS III represented according to the standard 96-condition screen layout. The screen is a 3D grid composed of 8 additive mixes (dipeptides, vitamins, nucleosides *etc.*), 4 cryoprotecting precipitant mixes (*e.g.* PEG 4000 with glycerol) and 3 buffer systems (pH 6.5, 7.5 and 8.5).

Can you tell us more about the small drug-like compounds used as additives?

Surprisingly, well known drug compounds, with a more or less wide scope of binding potency, were not found to be particularly well represented in the PDB, such as the anaesthetic lidocaine, the antimalarial quinine and the antibiotic ampicillin (found ordered in 0, 3 and 8 PDB macromolecular structures, respectively). The initial selection of additives could therefore not be strictly based on a PDB search. Instead, lists of phytochemicals (including quinine, menthol, caffeic acid *etc.*) and essential medicines (including notably antibiotics, see Fig. 3) were consulted. Other types of compounds were tested to complete the formulation, such as nucleosides (*e.g.* thymidine found in 44 PDB structures) and cholic acid derivatives (*e.g.* CHAPS, 57 structures). The selection had to be restricted to compounds that are soluble and stable enough in water (or ethanol solution) and, later, in the MORPHEUS conditions.

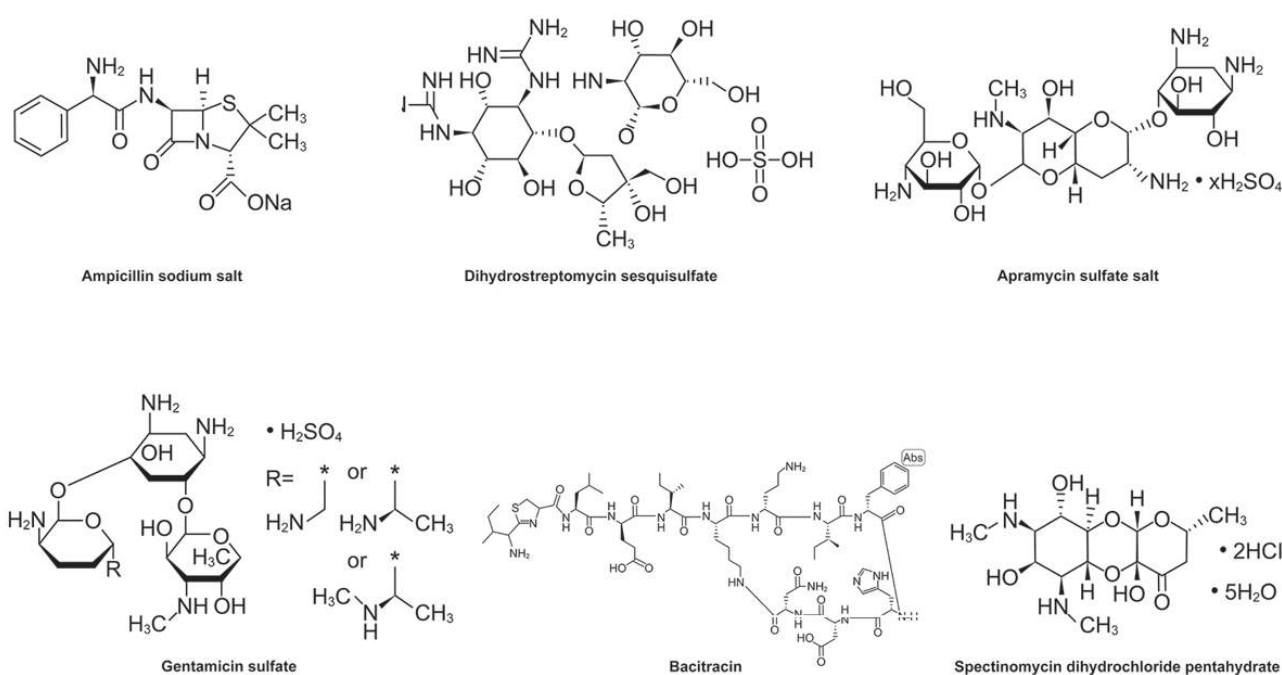


Figure 3. The 6 reagents forming the MORPHEUS III additive mix named 'Antibiotics' (conditions F1-F12). Note that bacitracin is an extraordinarily large compound (MW = 1422 Da) compared with all the other compounds used as additives in the screen (average MW = 248 Da).

Ultimately, cost-effectiveness had to be taken into account. It would be interesting to further develop the concept of combining crystallization and compound screening for specific drug targets, with (more costly) reagents adapted to advanced drug-design projects (Turnbull *et al.*, 2017).

Is MORPHEUS III more efficient than other crystallization screens?

MORPHEUS III was formulated to minimize the number of initial conditions employed (by integrating more reagents than traditionally used in each condition). In addition, the final choices of formulation are based on results from crystallization against a broad variety of novel samples produced at MRC-LMB. Consequently, the additives are not under-sampled and the screen is not biased towards a specific subset of protein samples.

Nonetheless, when facing unpredictability from a multitude of variables, 96 conditions are simply too few to cover the 'chemical space' efficiently. You should ideally proceed with many more conditions and different formulation strategies that complement each other. From this perspective, the relevance of MORPHEUS III was demonstrated when useful crystals were obtained that were not observed in many other screening kits (see Case study of MYC:MAX bHLHZip complex below).

Finally, what is the price of a novel macromolecular structure? The price of a structure with bound ligands? When an initial crystallization screen plays an essential part in the process, less time is spent on optimization of the sample, crystallization and crystal screening. This means a gain in effectiveness overall.

I would like to thank Jan Löwe and Olga Perisic (MRC-LMB) for their support in all aspects of this work. I also thank Jo Westmoreland (MRC-LMB, Visual Aids) and Rachel Kramer Green (PDB) for technical

support. LifeArc commercializes the MORPHEUS screens and derivative products (under exclusive licence to [Molecular Dimensions Ltd](#), Newmarket, UK).

Case study of MYC:MAX bHLHZip complex by Giovanna Zinzalla

Dr Zinzalla is currently an Assistant Professor in Chemical Biology at the Karolinska Institutet (Stockholm, Sweden). Her research is focused on determining how the MYC pleiotropic transcription modulator integrates fundamental processes required for proliferation and survival of normal and malignant cells. Her approach involves MYC structure-function studies and the use of chemical probes to modulate the MYC network of protein-protein interactions that coordinate the expression of a large and extremely diverse set of genes, with the ultimate goal of developing new therapeutics.

The basic helix-loop-helix leucine zipper (bHLHZip) region of MYC binds to the obligate-partner MAX. A better understanding of the MYC:MAX bHLHZip complex is essential for anticancer drug discovery (Soucek *et al.*, 2008; Zinzalla, 2016). Therefore, Giovanna has been carrying out extensive biophysical and structural studies on this complex (NMR and X-ray crystallography). Previously, this system has only been crystallized in the presence of DNA (Nair & Burley, 2003), the underlying reason being that the complex is very dynamic in the absence of DNA and hence particularly challenging to crystallize. For drug discovery purposes however, a crystal structure of the free form is essential in enabling the development of synthetic molecules that inhibit the MYC:MAX interaction and binding to DNA.

In an attempt to increase the yield of useful crystals for a sample of c-MYC:MAX bHLHZ, Giovanna employed an unusually large initial screen composed of 2112 initial conditions at the [MRC-LMB crystallization facility](#) (Gorrec & Löwe, 2018). The screen included the MORPHEUS kits, among many others. After an extensive crystal screening of the various hits obtained, it was observed that only the crystals from a MORPHEUS III condition enabled structure solution with 1.35 Å resolution (manuscript submitted).

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INTERVIEW

Edward Tiekink



The IUCr Newsletter asks IUCrData Editor Edward Tiekink about his career, his involvement with IUCr Journals and his predictions for crystallography.

Could you provide our readers with a short summary of your career to date, including main research interests and collaborations?

I graduated from University of Melbourne, Australia, obtaining my PhD degree in inorganic chemistry/crystallography in 1985, and am now a Distinguished Professor and Head of the Research Centre for Crystalline Materials at Sunway University in Malaysia. Prior to my current position, I spent 16 years at the University of Adelaide, Australia, before 'continent hopping', first to Singapore in 2001, then Texas, USA, and finally back to Asia in 2009, all this interspersed with short-term positions back in Australia and in Brazil. Wherever I have been, I have pursued my scientific passion for chemical crystallography and continued my work in developing metal-based drugs; in 2006 I was awarded a DSc from the University of Melbourne for this work.

During my career, I have seen crystallography as an academic pursuit nearly disappear, being relegated to 'service work' until the emergence of 'crystal engineering', which has heralded a new breed of crystallographer, often non-specialist. This downgrading of crystallographers was partly the motivation for leaving my position in Adelaide to join the Department of Chemistry at the National University of Singapore, where I was allowed to follow my scientific interests.

In Singapore, I delved more deeply into the fundamental question of molecular crystallography, how and why crystals form, specially looking at secondary interactions involving main group elements and later

more esoteric points of contacts between molecules such as $\text{Au}\cdots\pi$, $M(\text{lone-pair})\cdots\pi$, etc. Much of this work, certainly the fun part, has been conducted in collaboration with Ionel Haiduc (Romania), Julio Zukerman-Schpector and Ignez Caracelli (Brazil).

How did you become involved with the IUCr?

Being the overarching body for connecting crystallographers from all backgrounds, the running of major congresses and an impressive suite of journals, it is hard for a crystallographer not to be associated with the IUCr in some fashion. I guess my formal association arose in 2000 when Bill Clegg invited me to join the founding Editorial Board of a new journal, *Acta Crystallographica Section E*. This role developed into my appointment as a Section Editor in 2009. Now, my active participation with the IUCr revolves around yet another journal, *IUCrData*.

Acta E has undergone a number of changes recently. Can you explain briefly in your opinion how these changes will benefit the community?

I am convinced of the need for an outlet for medium-sized papers describing new structures, and the new format of *Acta E* clearly provides authors with this opportunity. At the same time, the opportunity to publish restricted reports has been retained by the emergence of *IUCrData*. My overarching concern is that all structures need to be properly refereed, especially as we rely on the Cambridge Structural Database so much in our research - who wishes to work with dodgy structures? As an author, the fear/favour no-one approach by Editors is reassuring and provides validation for data collection and refinement methodologies, which is really important when establishing new laboratories with different instruments, etc. The new format of *Acta E* gives authors opportunities to write about their work and delve into the structure more, often leading to new insights into (structural) chemistry.

What do authors need to be aware of before submitting to the journal now?

Authors should avail themselves of the [Notes for Authors](#). These have undergone refinement over the years and are an absolute must when preparing their submissions. The instructions are more of a guide and are easy to read, self-explanatory and even educational. The other thing authors should do is critically evaluate [checkCIF](#) reports and the [printCIF](#) outputs. Free access to the formatting program [publCIF](#) is a 'gift' to authors, being incredibly user-friendly.

Having published well over 800 papers across IUCr Journals, which have been your most memorable and why?

Wow! So many? In these days of metrics and all that, it might be tempting to mention a (relatively) highly cited paper, one describing the structure of Et_3PAuCl [*Acta Cryst.* (1989), **C45**, 1233-1234]. But no, a paper ranking high in my mind describes the structure of $\text{Cd}(\text{S}_2\text{COMe})_2$ [*Acta Cryst.* (2002), **E58**, m537-m539]. A culminated effort of over 20 years, actually probably longer, was spent in getting crystals of this compound, and the pieces of 'dust' I managed to grow were revealed by Victor Young Jr, employing synchrotron radiation, as a lovely one-dimensional coordination polymer. What really struck me then was that from data collection to the appearance of the structure in published form was only a matter of days - how things had changed!

If you had to gaze into a crystal ball, what would you predict being hot topic areas or techniques to look out for in the future?

I feel much molecular crystallography would benefit greatly by employing complementary spectroscopic and high-level computational techniques to explore issues such as nucleation, thermodynamics of crystal growth, etc., not to mention determining reliable assessments of energies of supramolecular association.

Studies in these areas are already under way but I feel more researchers will be attracted to these important topics.

HISTORY OF CRYSTALLOGRAPHY

How did they do that? Beevers-Lipson strips

Mike Glazer



Henry Solomon Lipson (1910-1991) (left) and Cecil Arnold Beevers (1908-2001) (right)

The idea of using Fourier methods in crystallography was first proposed by William Henry Bragg in his Bakerian Lecture of 1915, but it was his son William Lawrence Bragg, who first used this procedure in his determination of the structure of diopside in 1928. In W. L. Bragg's own words^[1]: *I tried hard to see how all the reflections around a zone could be used to build a two-dimensional Fourier projection on a plane, but I missed the answer. It was provided by my father. He had been thinking about the same problem and wrote to me on my return, showing how the Fourier series should be formed but asking my advice as to whether the coefficients should be intensities or amplitudes. I replied that they should be amplitudes, and that I had sets of them obtained from diopside ready for trial. I put these coefficients in the Fourier series, summed it up, and behold there were the calcium, magnesium, silicon and oxygen atoms clearly shown by peaks in the Fourier summation. I wrote to my father with much excitement, and proposed that we should write a joint paper about it. He insisted that I should write it up alone, but I have always regretted that I agreed to do so. The idea as to how the Fourier series should be summed was entirely his, and I think he felt sad that the first paper describing its use should appear over my name. He should have published the idea, and I should have published its application to diopside. It was in this year that West and I published a paper on the analysis of structures with many parameters in which we summarised all we had learnt about techniques.*

It was soon realized that in order to solve crystal structures of ever more complexity crystallographers would need to be able to add together huge numbers of trigonometric terms. The aim of adding Fourier terms is to produce maps showing electron density (in the case of X-rays) within a unit cell. I think it is worth looking back to understand how the early crystallographers tackled this problem, because then one can begin to appreciate just how clever they were in a much less technologically able world. Recall that until the 1960's the only practical way to find values of sines and cosines was by looking them up in printed tables or by the use of slide rules. No computers were available, nor calculators capable of computing trigonometric terms. Today, Fourier summation is taken for granted, and what used to take weeks to carry out can now be done in the blink of an eye. So how did they do it?

The story begins in Liverpool University with the collaboration of two research students, Cecil Arnold Beevers (1908-2001) and Henry Solomon Lipson FRS (1910-1991)[ii]. It had been proposed to them by a member of staff that they might like to work on the solution of crystal structures using X-ray diffraction. However, the availability of equipment then at Liverpool was limited and so the two students decided to approach W. L. Bragg at Manchester University for help. Bragg gladly agreed to help them, giving them access to his ionization spectrometer (a forerunner of the modern diffractometer), originally invented by his father. He also assigned one of his own students, Will Taylor[iii], to help them. In Lady Bragg's words: *I remember how Lipson with his colleague C. A. Beevers, as young students working in Liverpool, used to come over to Manchester with their current crystal model to get help over the structure, and how Beevers used to bicycle all the way to save the fare.*

Lipson and Beevers started to use Fourier techniques to solve the difficult case of the structure of copper sulfate pentahydrate[iv], the main problem being that the structure is of low symmetry in space group

$$P\bar{1}$$

and so the oxygens are not located on special positions. Beevers calculated that the time taken to use 90 terms in two dimensions for calculation of a single point of electron density on a grid of 1000 points was about 90 minutes. At their present rate the work would have taken about one year to complete! It was then on 4 December 1933 that Lipson had a brainwave. To understand this recall that a two-dimensional electron-density projection on (001) can be expressed by a sum of Fourier terms thus:

$$\rho(x, y) = \frac{1}{A} \sum_h \sum_k F(hk0) \cos[2\pi(hx + ky)]$$

(1)

Lipson realized that this equation could be reformulated as:

$$\rho(x, y) = \sum_h \cos 2\pi hx \left[\sum_k \frac{F(hk0)}{A} \cos 2\pi ky \right] - \sum_h \sin 2\pi hx \left[\sum_k \frac{F(hk0)}{A} \sin 2\pi ky \right]$$

(2)

which can then be written simply thus:

$$\rho(x, y) = \sum_h P(k) \cos 2\pi hx - \sum_h Q(k) \sin 2\pi hx$$

(3)

For a centrosymmetric structure:

$$P(k) = \pm \sum_k \frac{|F(hk0)|}{A} \cos 2\pi ky$$

$$Q(k) = \pm \sum_k \frac{|F(hk0)|}{A} \sin 2\pi ky$$

(4)

Similar expressions can be constructed for non-centrosymmetric crystal structures. The book[v] by Kathleen Lonsdale, if you can find it, deals with this well. This separation into separate one-dimensional summations along x and y directions made a huge reduction in calculation time. The idea was first published in 1934 in a paper entitled 'A rapid method for the summation of two-dimensional Fourier series'[vi]. Lipson then began writing down the cosine and sine solutions onto strips of paper at home with the help of his mother. There were originally 2079 cosine strips and 1980 sine strips at 6° intervals, but later strips were produced at 3° intervals to increase the resolution. How many of us today would have the patience to do this?

Each 6° strip then represented values for:

$$A \cos 2\pi k(m/60) \text{ and } A \sin 2\pi k(m/60)$$

where **A** is an amplitude. To understand how to interpret such strips consider the following examples of cosine strips for $k = 8$ and $k = 13$.

29	C	8	29	19	$\overline{3}$	$\overline{23}$	$\overline{28}$	$\overline{14}$	9	26	26	9	$\overline{14}$	$\overline{28}$	$\overline{23}$	$\overline{3}$	19	29
$\overline{43}$	C	13	$\overline{43}$	$\overline{9}$	39	25	$\overline{29}$	$\overline{37}$	13	43	4	$\overline{41}$	$\overline{21}$	32	35	$\overline{17}$	$\overline{42}$	0

On the first strip, the first number represents the value of the amplitude **A** = 29. The back of the strip has the value for -29. The second strip is for an amplitude of -43. In total, amplitudes were given up to a value of ± 99 . The letter C tells us that these are cosine strips and the following number, 8 or 13, is the value of k . There then follow 16 values corresponding to the index m from 0 to 15. As this covers one quarter of a cycle, the symmetry of the trigonometric function is used to find the values in subsequent quarters. For the next quarter one simply reverses the order.

Now in order to compute a Fourier summation, we start with a value for h , and all the strips corresponding to the different values of k are selected from the cosine box, and then laid one above the other on the table. It is then necessary to add the numbers down each column to obtain values for $P(k)$. Then other values of h are chosen and the exercise repeated. This is repeated for strips taken from the sine box to obtain values of $Q(k)$.

Let's take, as a simple example, the following set of structure factors with $h = \pm 1$ obtained by X-ray diffraction for a certain centrosymmetric cubic structure (the full table, not shown here, would list the structure factors for h and $k = 0, \pm 1, \pm 2, \pm 3, \dots$).

Table 1. Structure factors

h	k	$\pm F /A$	Multiplicity
0	1	-4	2
0	2	28	2
0	3	-9	2
1	0	-4	2
1	1	21	4
1	2	-4.5	4
1	3	15.5	4
2	0	28	2

2	1	-5	4
2	2	23	4
2	3	-5	4
3	0	-9	2
3	1	15	4
3	2	-5	4
3	3	13	4

As this is centrosymmetric cubic we can write:

$$F(hk0) = F(\bar{h}\bar{k}0)$$

So, in order to deal with positive and negative values of h we calculate

$$A_1 = [F(hk0) + F(\bar{h}\bar{k}0)] \quad \text{and} \quad A_2 = [F(hk0) - F(\bar{h}\bar{k}0)]$$

in order to tabulate values of $P(k)$ and $Q(k)$, respectively. In this case, $Q(k) = 0$, and so there are no sine terms to consider.

This will be used as part of a (001) projection of the structure. We choose five strips from the cosine box and carry out the summations $P(k)$ with $k = 0, 1, 2, 3, 4$ and taking $h = 1$.

Evaluation of $\sum_k A_1 \cos 2\pi ky$ for $h = 1$

m	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	
$\bar{8} \text{ C } 0$	$\bar{8}$	$\bar{8}$	$\bar{8}$	$\bar{8}$	$\bar{8}$	$\bar{8}$	$\bar{8}$	$\bar{8}$	$\bar{8}$	$\bar{8}$	$\bar{8}$	$\bar{8}$	$\bar{8}$	$\bar{8}$	$\bar{8}$	$\bar{8}$	(-128)
$\bar{18} \text{ C } 2$	$\bar{18}$	$\bar{18}$	$\bar{16}$	$\bar{15}$	$\bar{12}$	$\bar{9}$	$\bar{6}$	$\bar{2}$	2	6	9	12	15	16	18	18	(0)
	$\bar{26}$	$\bar{26}$	$\bar{24}$	$\bar{23}$	$\bar{20}$	$\bar{17}$	$\bar{14}$	$\bar{10}$	$\bar{6}$	$\bar{2}$	1	4	7	8	10	10	
$84 \text{ C } 1$	84	84	82	80	77	73	68	62	56	49	42	34	26	17	9	0	(843)
$62 \text{ C } 3$	62	59	50	36	19	0	$\bar{19}$	$\bar{36}$	$\bar{50}$	$\bar{59}$	$\bar{62}$	$\bar{59}$	$\bar{50}$	$\bar{36}$	$\bar{19}$	0	(-165)
	146	143	132	116	96	73	49	36	6	$\bar{10}$	$\bar{20}$	$\bar{25}$	$\bar{24}$	$\bar{19}$	$\bar{10}$	0	
Sum	120	117	108	94	76	56	35	16	0	$\bar{12}$	$\bar{19}$	$\bar{21}$	$\bar{18}$	$\bar{11}$	$\bar{1}$	10	(551)

In practice, it was easy to make mistakes in the summations, and so it was usual to calculate checksums by totalling each row of values and comparing with the final row listing (illustrated here in bold at the right). The sums in this case correspond to values of $P(k)$. These sums are then used in

$$\rho(x, y) = \sum_h P(k) \cos 2\pi hx$$

to get the electron density at all points x and y (see Table 2).

Table 2. Evaluation of $P(k) \cos 2\pi hx$ at x from 0 to 15/60 and $h = 1$

	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
120 C 1	120	119	117	114	110	104	97	89	80	71	60	49	37	25	13	0
117 C 1	117	116	114	111	107	101	95	87	78	69	59	48	36	24	12	0

	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
108 C 1	108	107	106	103	99	94	87	80	72	63	54	44	33	22	11	0
94 C 1	94	93	92	89	86	81	76	70	63	55	47	38	29	20	10	0
76 C 1	76	76	74	72	69	66	61	56	51	45	38	31	23	16	8	0
56 C 1	56	56	55	53	51	48	45	42	37	33	28	23	17	12	6	0
35 C 1	35	35	34	33	32	30	28	26	23	21	18	14	11	7	4	0
16 C 1	16	16	16	15	15	14	13	12	11	9	8	7	5	3	2	0
0 C 1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-12 C 1	-12	-12	-12	-11	-11	-10	-10	-9	-8	-7	-6	-5	-4	-2	-1	0
-19 C 1	-19	-19	-19	-18	-17	-16	-15	-14	-13	-11	-10	-8	-6	-4	-2	0
-21 C 1	-21	-21	-21	-20	-19	-18	-17	-16	-14	-12	-11	-9	-6	-4	-2	0
-18 C 1	-18	-18	-18	-17	-16	-16	-15	-13	-12	-11	-9	-7	-6	-4	-2	0
-11 C 1	-11	-11	-11	-10	-10	-10	-9	-8	-7	-6	-6	-4	-3	-2	-1	0
-1 C 1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	0	0	0	0	0
10 C 1	10	10	10	10	9	9	8	7	7	6	5	4	3	2	1	0

The above table lists the electron-density contribution from reflections with $h = 1$ to all points in the Fourier map where x goes from 0 to 15/60.

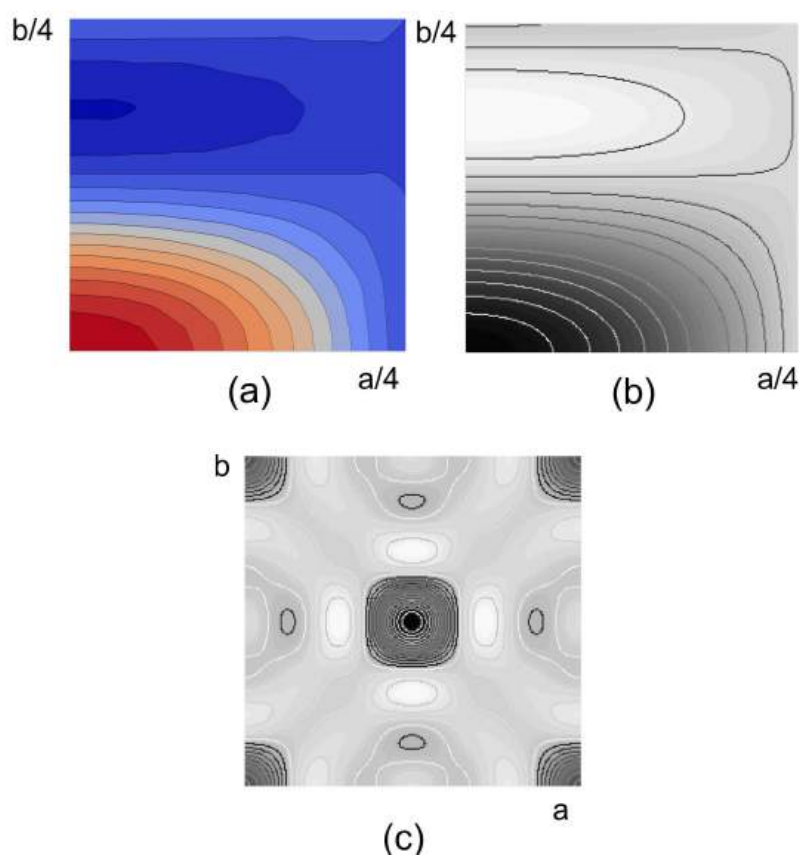


Figure 1. Fourier summation (from program *FOURIER2D*[vii])

Figure 1 shows a contour plot with just $h = 1$ made from the numbers in Table 2. The range of plot in each direction is from 0 to $\frac{1}{4}$ of the unit cell. This can be compared with Figure 1(b) which is an actual Fourier plot made with a modern Fourier plotting computer program using all the structure factors in Table 1, thus agreeing with our Beevers-Lipson calculation. Now, in order to obtain a complete Fourier plot it is necessary carry out the above procedure with all the values of h , i.e. with $h = 0, 1, 2, 3, \dots$. Figure 1(c) shows the effect of adding the cosine fringes for a full set of structure factors for h, k from 0 to ± 3 to get $\rho(x, y)$. We thus obtain a low-resolution map of the electron density of a cubic perovskite structure. Further details on how the strips were used can be found in the books by Lipson & Cochran[viii] and by Woolfson[ix]. Note, in passing, that by using $|F(hk0)|^2$ with strips from the cosine box alone, a Patterson map can be obtained. As can be seen, despite the simplification in equation (2), the process of using the strips was still complicated and time consuming.

Although the use of the strips cuts down the time factor enormously, I recall that when I started as a research student of Kathleen Lonsdale, together with the late Howard Flack, we were given a box of strips to compute a simple projection of hexamethylbenzene as an exercise. Even working together this took us a week to understand the process and then to obtain a low-resolution map! Restoring all the strips back into the box also took some considerable time. This exercise brought home to us just how much work was involved in computing Fourier maps before computers were widely available, and made us have considerable respect for the early crystallographers.

The idea for making available boxes of strips was published in 1936[x], in a paper in which Beevers and Lipson wrote: *We should be glad to know if workers in other laboratories who employ the Fourier method would find these strips useful, as it may be possible for the supply of copies.*

The publication of the so-called Beevers-Lipson strips caught on very quickly and around 500 sets were produced and exported all over the world and were in use even up to the 1970's. This was originally funded by a loan of £200 arranged by W. L. Bragg, in those days a considerable sum of money. Figure 2 shows the only remaining prototype box (cosine), which is in my possession, from which the others were derived. Unfortunately, the other box (sine) was thrown away by a colleague, before I could rescue it, during the move from the old Cavendish Laboratory to the new site in West Cambridge in 1974. Apparently, the original strips were written mainly at Lipson's home in the kitchen with his mother copying the negative amplitude numbers on the backs of the positive amplitude strips. I recently examined the strips closely and found that some were handwritten in pencil (see Figure 3) perhaps by Lipson's mother!



Figure 2. Prototype 6° cosine box of Beevers-Lipson strips. The boxes exported to other laboratories had sloping sides to ensure that when a strip was removed its place was left open for its re-insertion.

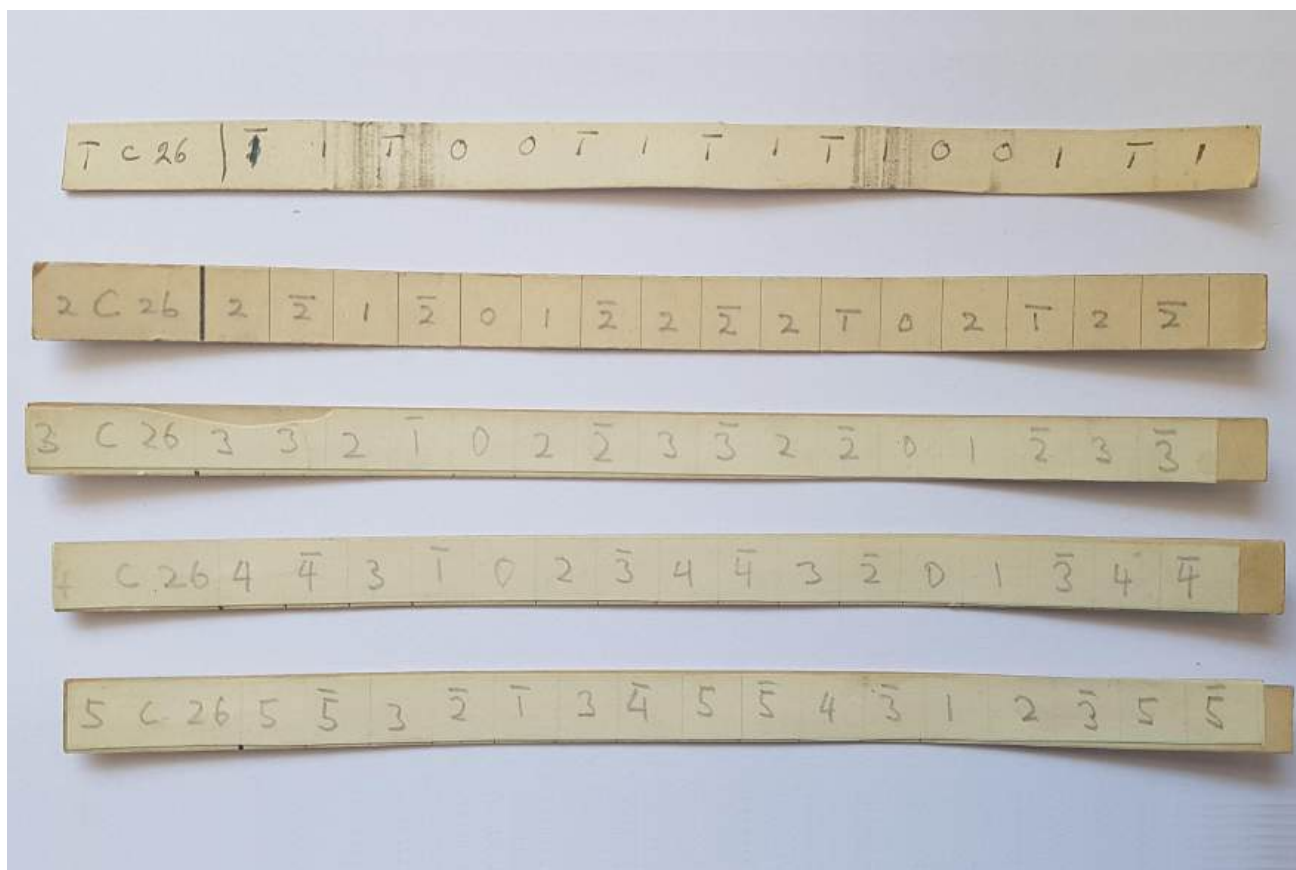


Figure 3. Some examples of handwritten Beevers-Lipson strips from the prototype cosine box.

Figure 4 shows Beevers together with Lipson's daughter Ann bathing in the sea during the 1951 IUCr Congress of Crystallography in Stockholm. This was one of two photographs that came to be known as 'Beevers-Lipson stripped'!



Figure 4. Beevers-Lipson stripped! (with thanks to Ann Lipson, deceased March 2017).

The boxes of Beevers-Lipson strips were used extensively to solve many important crystal structures. For example, the solution of the structure of penicillin by the Nobel Prize winner Dorothy Hodgkin was made possible by using the strips in order to create Fourier and Patterson maps showing the atomic positions. A look through copies of *Acta Crystallographica* from 1948 shows many examples of structures and Fourier maps made with Beevers-Lipson strips.

I should record here that Lipson went on to make many important contributions to crystallography. For instance, and largely forgotten, he showed with a student Vera Daniel in 1942 that extra powder lines observed in an alloy of copper, iron and nickel by A. J. Bradley could be interpreted in terms of having a modulated (or in today's terminology incommensurate) structure, see Figure 5.



Figure 5 Extra side-band powder diffraction lines observed in a Cu, Fe, Ni alloy by Daniel & Lipson in 1942[xi].

Figure 6 shows a photograph of Henry Lipson, Margaret Farquhar and Will Taylor in the Cavendish Laboratory in 1945. Lipson and Farquhar[xii] worked on the determination of precise lattice constants from powder diffraction. In 1957, Lipson was elected Fellow of the Royal Society.

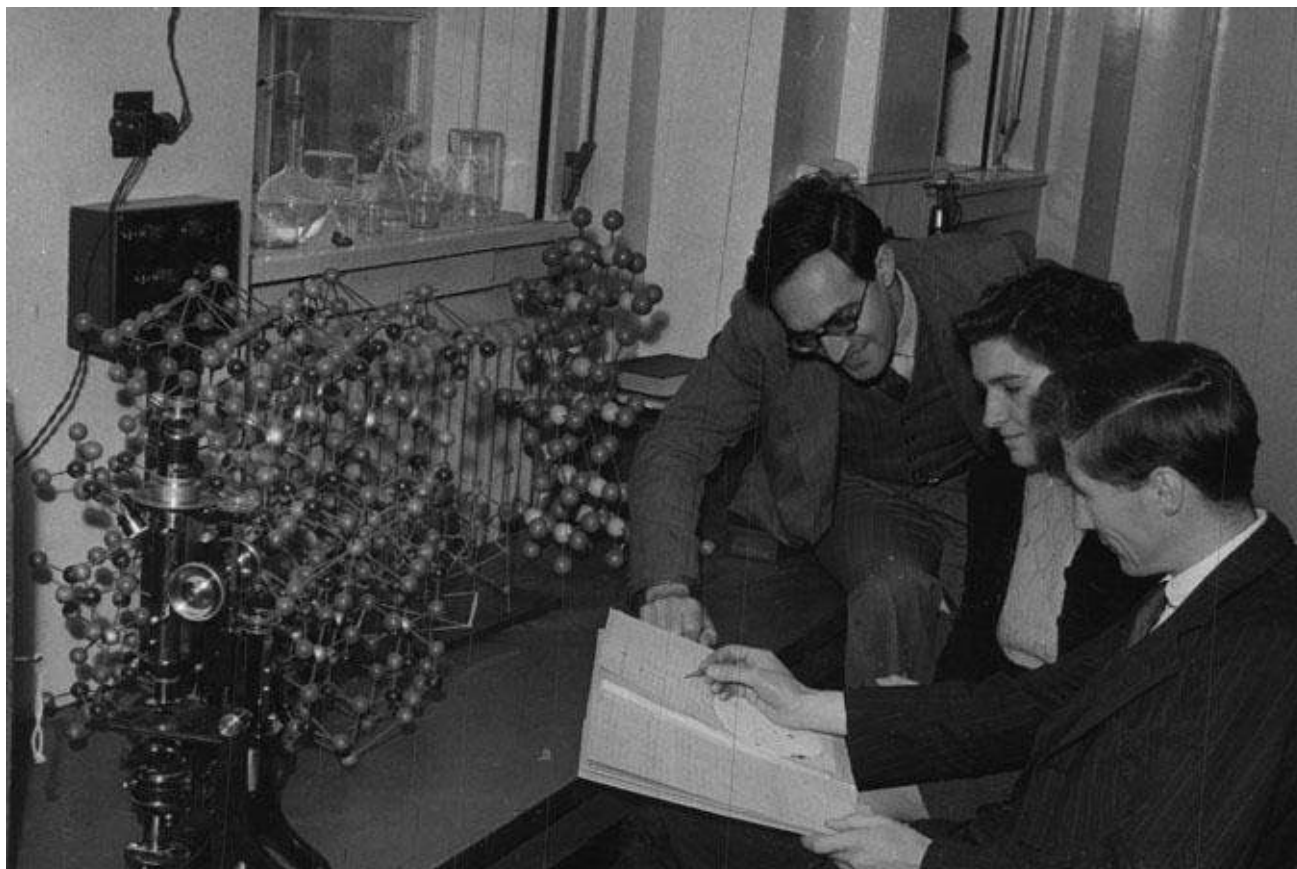


Figure 6. H. S. Lipson, Margaret C. M. Farquhar, W. H. Taylor: Austin Wing, Cavendish Laboratory, Cambridge 1945.

In 1938 Beevers became Dewar Fellow in Crystallography at the [University of Edinburgh](#), a post jointly associated with the Departments of Physics and Chemistry. Beevers was elected a Fellow of the [Royal Society of Edinburgh](#) later in the same year. He remained in [Edinburgh](#) for the rest of his life and was Reader in Crystallography at the University.

Arnold Beevers was a Quaker and this influenced his approach to life and science. He set up a company employing disabled workers. This was called Beevers Miniature Models (now Miramodus Ltd), which produced ball-and-spoke crystal structure models. It was possible to purchase completed models or to buy sets of miniature plastic balls (we used to call them Beevers' balls) in order to construct one's own models. Arnold was genial and a delightful entertainer. A famous joke that he used to play at conference dinners was to get the audience to sing the song 'My Bonnie Lies Over the Ocean' during which everyone had to stand up or sit down every time a word beginning with the letter B was sung. I well remember his invited lecture on crystal models at the IUCr Congress in Hamburg in 1984. Only Arnold could talk on such a topic and keep the audience entertained for such a long time.

[i] *Crystal Clear: The Autobiographies of Sir Lawrence and Lady Bragg*, edited by A. M. Glazer and P. Thomson, published by Oxford University Press (2015).

[ii] M. M. Woolfson, *Biogr. Mem. Fell. R. Soc.*, **39**, 228-244 (1994).

[iii] William (WHT) Hodge Taylor (1905-1979) had been a graduate student of WLB in 1926 and remained in Manchester until 1934. He then went to Cambridge to work with J. D. Bernal and then to the Davy-Faraday Laboratory to work under W. H. Bragg, before returning in 1936 to Manchester as Head of the Physics Department of the College of Technology. He was the first person to make a full description of the crystal structures of feldspars in 1933, one of the most common minerals on earth (and later found on the moon). He later moved to the Cavendish Laboratory in Cambridge with William Lawrence Bragg and

was instrumental in running the newly created Crystallography Laboratory, where he remained until his retirement in 1971.

[iv] The same compound used to obtain the first X-ray diffraction photograph by Friedrich and Knipping in the Spring of 1912.

[v] K. Lonsdale. *Crystals and X-rays*. Bell & Sons (1948).

[vi] C. A. Beevers and H. Lipson. *Phil. Mag.* **17**, 855-859.

[vii] A. M. Glazer. *J. Appl. Cryst.* **49**, 2276-2278 (2016).

[viii] H. Lipson and W. Cochran. *The Determination of Crystal Structures*. Bell & Sons (1966).

[ix] M. M. Woolfson. *An Introduction to X-ray Crystallography*. Cambridge University Press (1970).

[x] C. A. Beevers and H. Lipson. *Nature*, **137**, 825-826 (1936).

[xi] V. Daniel and H. Lipson. *Proc. Roy. Soc. A*, **181**, 368-378 (1943).

[xii] M. C. M. Farquhar and H. Lipson. *Proc. Phys. Soc.* **58**, 200 (1946).

OBITUARY

Yukiteru Katsube (1930-2016)

Tomitake Tsukihara



Yukiteru Katsube. Photo courtesy of the *Journal of the Crystallographic Society of Japan*.

Yukiteru Katsube, Professor Emeritus at Osaka University, Japan, died on 1 April 2016 in Osaka at the age of 85. He was a leader in protein crystallography in Japan.

Professor Katsube was born in Yonago, Japan, on 3 November 1930. He graduated from Himeji Institute of Technology, Japan, in 1953, and worked as a Research Associate there until 1957, when he entered the Graduate School of Engineering of Osaka University. He was an Associate Professor of Himeji Institute of Technology (1959-1966) and Tottori University, Japan (1966-1971), and a Professor of Tottori University (1971-1983). He joined the Institute for Protein Research (IPR) of Osaka University in 1983, and served as Director of the Institute from 1988 to 1992.

He initiated crystal structure analysis of a tetrapeptide, glycyl-L-prolyl-L-leucyl-glycine, by the vector-seeking method. In 1967, he successfully determined its structure by the heavy-atom method [Ueki *et al.* (1967). *Nature* **216**, 1205].

He led the crystallographic group in Tottori University, where he determined a series of metabolite structures of *Aspergillus*, with the goal of understanding metabolic pathways. He successfully applied the anomalous dispersion effect of oxygen atoms to determine their absolute configurations, which are key to determining their metabolic pathway.

His first achievement in protein crystallography was solving the structure of algal [2Fe-2S] ferredoxin [Fukuyama *et al.* (1980). *Nature* **286**, 522]. In addition, he determined a novel structure of bacterial

[4Fe-4S] ferredoxin by the native anomalous dispersion method using Cu K α rays [Fukuyama *et al.* (1988). *J. Mol. Biol.* **199**, 183], thus making an important contribution to research on the molecular evolution of iron-sulfur proteins.

As the leader of protein crystallography at IPR from 1983 onward, he introduced molecular biology technology to protein crystallography to elucidate the structure-function relationships of proteins. He collaborated with biologists in various fields and determined many protein structures, e.g. xylanase, cyclodextrin glucanotransferase, 1,6-glucosidase, β -amylase, 3-isopropylmalate dehydrogenase, hydroxylamine oxidoreductase, Cu/Zn-superoxide dismutase, Mn-superoxide dismutase, tryptophanase, glutathione synthetase and basic fibroblast growth factor. He introduced many biochemists to structural biology, and trained many young structural biologists who continue to be active in research today.

He served on the Editorial Advisory Board of *Acta Crystallographica Section D* and the advisory board of the BNL Protein Data Bank.

After retiring in March 1993, he made every effort to spread protein crystallography to private companies. He was the Senior Advisor to the President of Rigaku Corporation (1996-2003), the Chairman of PharmaAcess Inc. (2003-2015) and the President of Protein Mall Kansai (2009-2015). Despite his declining lung function over the past few years, Professor Katsube eagerly performed these duties. After many long years of productive contributions to science, his life has come to an end. May his soul rest in peace.

OBITUARY

Ted Janssen (1936-2017)

Bernd Souvignier



Theo Willem Jan Marie (Ted) Janssen passed away on 29 September 2017 in Groesbeek. He was born on 13 August 1936 in Vught, near 's-Hertogenbosch. Together with Pim de Wolff and Aloysio Janner he was one of the founding fathers of N -dimensional crystallography, more specifically of the superspace approach, in which structures with sharp diffraction peaks but lacking three-dimensional lattice periodicity are indexed using $N > 3$ indices.

After studying theoretical physics in Utrecht, graduating under Leon van Hove, he met Aloysio Janner in 1965 and became his first PhD student at the Radboud University in Nijmegen (then still called the Catholic University Nijmegen). He finished his PhD thesis, *Crystallographic Groups in Space and Time*, in 1968, thereby providing the theoretical basis of what would become the superspace approach. In 1972, he was appointed as an Associate Professor in Nijmegen and became promoted to full Professor of Theoretical Physics in 1995.

Ted's PhD thesis already showed his deep understanding of the mathematics underlying the symmetry analysis of physical structures. For example, he applied abstract cohomology theory to describe space groups as group extensions of the translation subgroup by the point group and it is not surprising that (besides acknowledging, for example, the support of Edgar Ascher) Ted thanks several mathematicians for helpful discussions. This clearly illustrated Ted's truly interdisciplinary scientific position, interacting with physicists as easily as with mathematicians and materials scientists.

At the IUCr Congress in Kyoto in 1972, Ted and Aloysio Janner met Pim de Wolff from the Delft University of Technology, who presented his work on incommensurately modulated crystals, which he proposed to describe in a four-dimensional space. They recognized that the corresponding four-dimensional symmetry groups were precisely the same as the space-time groups occurring in their own work, and from then on the three joined forces to generalize the superspace approach to other aperiodic structures such as composite structures and quasicrystals (which were discovered in 1982). The groundbreaking importance of the superspace approach was acknowledged by the award of the Aminoff Prize of the Swedish Academy of Science to Ted, Pim de Wolff and Aloysio Janner in 1988 and the Ewald Prize of the IUCr to Ted and Aloysio in 2014. Their contributions were also explicitly mentioned when the Nobel Prize for Chemistry was awarded to Dan Shechtman in 2011 for the discovery and description of quasicrystals.

From Ted's appointment as a staff member in Nijmegen in 1972 onwards, he and Aloysio created a strong group in solid-state physics, including experimentalists but also reaching far into the mathematics department. The interdisciplinarity of the group corresponded to the impressively broad range of research topics to which Ted made substantial contributions. On the one hand are his famous publications on the mathematical description of quasicrystals, on the other hand one finds his work in collaboration with experimentalists, looking at vibrational modes of phonons, phason modes (in relation to sliding modes and frictionless motion) and the analysis of phase transitions in aperiodic structures (with original publications as late as 2011).

Ted's research articles show an extraordinary combination of clear style and precision. Listening to his scientific talks was always a pleasure and his eagerness to share his knowledge made him an inspiring lecturer, giving well received courses on a broad range of topics including quantum mechanics, chaos theory, mathematical physics and group theory. Some of his excellent syllabi were adopted by his fellow lecturers and have even been in use at Radboud University long after Ted's retirement. His monograph *Crystallographic Groups* is still one of the best resources on this topic, both covering the mathematical background with the required precision and demonstrating its application to real physical phenomena.

Ted served the scientific community in various roles, including as an editor (he was a Co-editor for *Acta Crystallographica Section A* from 1993 to 2002), as a reviewer and as Chair of IUCr *ad hoc* Commissions on Nomenclature. In 1996, he submitted a proposal for a Volume A2 of *International Tables for Crystallography*, devoted to *N*-dimensional crystallography. Although this volume was never realized, the content of the proposal is remarkable, as it suggested a computer-based approach, generating the requested information by a collection of algorithms from a database of stored information. The ideas in this proposal have since been realized in the Bilbao Crystallographic Server.

During the restructuring of the Faculty of Science at Radboud University, Ted played an active role in setting up a group on Theoretical Condensed Matter within the newly founded Institute for Molecules and Materials (IMM). Even after his retirement, he was frequently present at the Institute's seminars, and was always ready to help with scientific questions or requests and happily gave talks himself.

Besides his scientific interests, Ted was very interested in the arts, enjoying literature, the visual arts and especially music. Throughout his life he took great pleasure in playing the piano, harpsichord and cello.

We have lost a great colleague and we will honour his memory if we keep our scientific interests as broad, multi-layered and interdisciplinary as Ted's were.

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AWARDS AND PRIZES

IUCr Executive Committee member honoured



Jenny Martin, pictured at an IUCr Executive Committee meeting at the Hyderabad Congress in 2017.

Jenny Martin, Director of the Griffith Institute for Drug Discovery at Griffith University in Brisbane, Australia, President of the Asian Crystallographic Association, and member of the IUCr Executive Committee, has been made a Companion of the Order of Australia (AC) in the Australia Day Honours List.

Professor Martin is a renowned protein crystallographer and structural biologist, as well as a former Editor of *Acta Crystallographica Section D*. Professor Martin has focused on the structure determination of disease-causing proteins to aid the design of new drugs that can combat them. Her work in this field has also been recently recognised by her election to the Australian Academy of Science, her election as an Eminent Fellow of the Royal Australian Chemical Institute and her elevation to Bragg Member of the Royal Institution of Australia. She is a relentless champion for gender equality, as reflected in her being awarded the Wunderly Oration Medal from the Thoracic Society of Australia and New Zealand.

Professor Martin AC was overwhelmed by the award and the public response (including trending on Twitter in Australia), saying 'I was thrilled, humbled and shocked in equal measure. The award of an AC is a rare privilege and I am enormously grateful to whoever nominated me. It's wonderful recognition of my work, my leadership in crystallography and drug discovery, and the values that I hold dear - excellence, respect, integrity, collegiality and authenticity.'

Additional reading

Griffith University News

<https://app.secure.griffith.edu.au/news/2018/01/26/top-australia-day-honour-for-griffith-science-leader/>

ABC National (featured on News breakfast, national news and online)

<http://www.abc.net.au/news/2018-01-26/meet-the-recipients-of-this-years-australia-day-honours-list/9362414>

Courier Mail

<http://www.couriermail.com.au/news/queensland/australia-day-honours-top-queenslanders-among-recipients/news-story/c253129cb2a3a2da12e73bb44ad98a74>

Australian Associated Press

<http://www.news.com.au/finance/work/leaders/calls-for-greater-diversity-in-australia-day-honours/news-story/b02c5c46fd32d61ff9b0282ceffb9bba>

Sydney Morning Herald

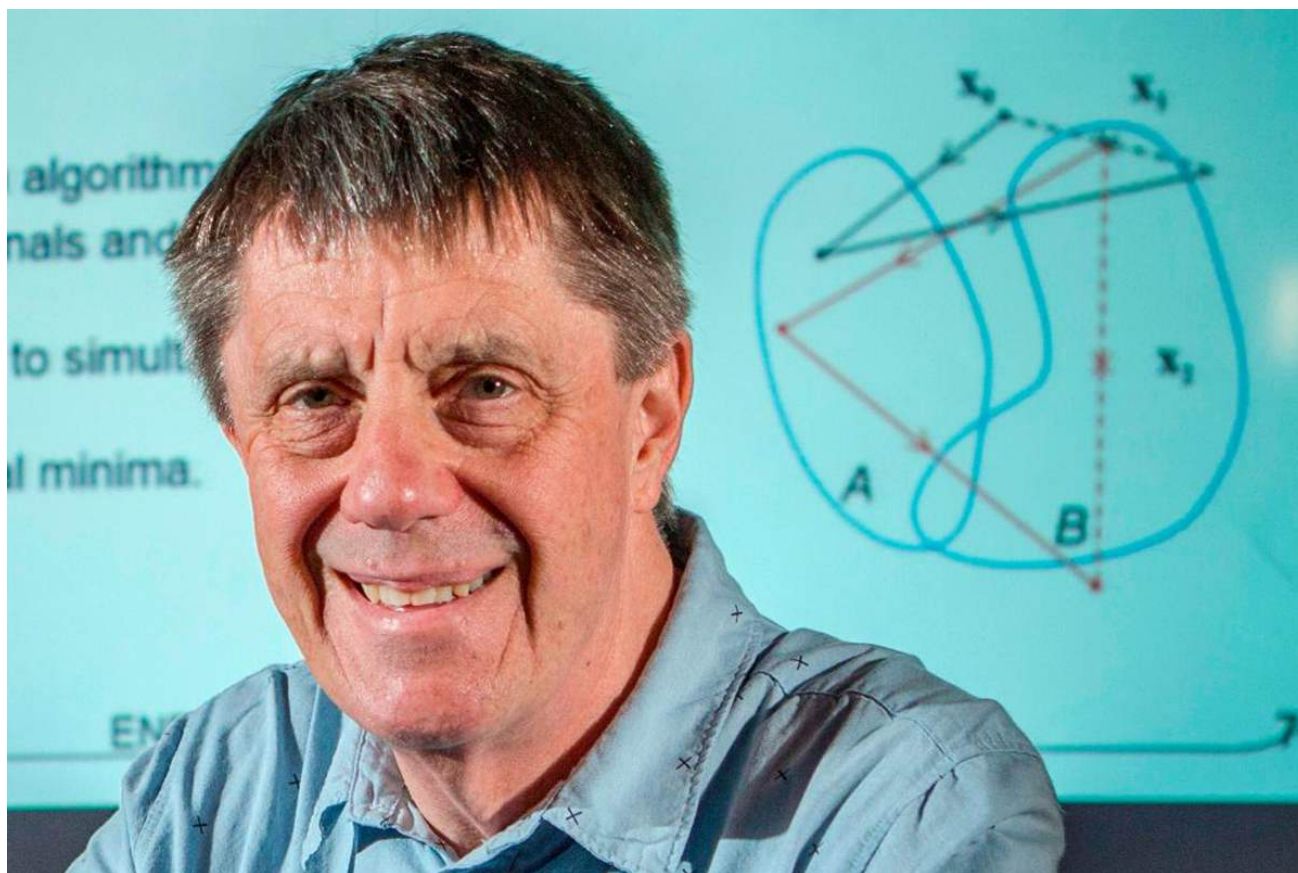
<http://www.smh.com.au/comment/australia-day-honours-dave-and-john-aplenty-but-women-are-in-the-wings-20180125-h0o8da.html>

Australian Academy of Science

<https://www.science.org.au/news-and-events/news-and-media-releases/fellows-recognised-in-australia-day-honours>

AWARDS AND PRIZES

Rick Millane elected as Fellow of the Royal Society Te Apārangi



Rick Millane. Photo courtesy of U. of Canterbury, Christchurch, New Zealand.

Former *Acta Crystallographica Section A* co-editor Rick Millane (University of Canterbury, Christchurch, New Zealand) has been elected as a Fellow of the Royal Society Te Apārangi. The fellowship recognises true international distinction in research and scholarship for advancing science, technology and the humanities. Professor Millane's theoretical and computational methods for imaging biological molecules and tissue using X-rays and optical radiation allow their structures to be determined, which is key to understanding disease, for drug design and for non-invasive medical imaging.

In 2017, Professor Millane was one of an international team of researchers awarded a NZ\$2 million research grant by the Human Frontier Science Program (to develop a novel method for imaging individual biomolecules with atomic resolution).

In late 2016, he was awarded the T. K. Sidey Medal from the Royal Society Te Apārangi for his contributions to methods for imaging biological molecules. In 2012, he became the first New Zealander to be named a Fellow of SPIE, the international society for optics and photonics, for his achievements in diffraction and reconstruction algorithms for biophysical imaging.

Professor Millane is well known internationally for his work on 'phase-retrieval' methods, an important component of X-ray diffraction imaging, publishing his first papers in this area in the early 1990s. His phase-retrieval algorithms have been applied to the latest imaging technology: X-ray free-electron lasers (XFELs), which use X-ray pulses short enough and intense enough to image biomolecules that have defied conventional imaging methods, and use nano-scale crystals with just a few unit cells in each

direction. This technology has the potential to greatly advance understanding of disease processes and drug design. He is acknowledged as a leader in advancing algorithms that are suitable for this new technology. He was also awarded a prestigious James Cook Research Fellowship in 2012 from the Royal Society of New Zealand to work on this topic.

Professor Millane has also worked on fibre diffraction analysis for imaging and determining the structures of disordered or non-crystalline substances, including biopolymers such as DNA and sugars in connective tissue. His work on optical diffusion imaging has contributed to a new non-invasive medical imaging technique.

Professor Millane has published widely in IUCr Journals. You can see a full list of papers [here](#).

Breaking news

Professor Millane has been announced as the recipient of the University of Canterbury's Research Medal 2018, one of the highest awards the University's Council can bestow. "Professor Millane is recognised as an outstanding researcher, educator and educational leader. His skills are diverse and his work is interdisciplinary," said Deputy Vice-Chancellor | Tumu Tuarua and chair of the Selection Committee, Ian Wright. The 2018 medal will be officially presented to Professor Millane by the UC Chancellor | Te Kumu Kaunihera, John Wood, later this year at the Chancellor's Dinner.

AWARDS AND PRIZES

Richard Henderson receives royal recognition



Richard Henderson (right) with Gautam Desiraju, LOC Chair, at IUCr2017.

IUCrj Editorial Board Member Richard Henderson (MRC LMB, Cambridge, UK) has been made a Companion of Honour in Queen Elizabeth II's 2018 Birthday Honours list for services to electron microscopy of biological molecules. The order is a special award held by only 65 people at any one time.

The Editor-in-Chief of IUCr Journals, Samar Hasnain, congratulated Richard on behalf of the editorial management board: 'Richard deserves this special recognition as he has served the community over a long period, influencing younger and senior colleagues alike with his infectious enthusiasm and passion for science. I and the Union are grateful for his tremendous hard work in helping to make cryo-electron microscopy (cryoEM) one of the main features of our journals, particularly **IUCrj**, as well as the IUCr Congress held in Hyderabad last year.'

In 2017, Richard shared the Nobel Prize in Chemistry for developing cryoEM for the high-resolution structure determination of biomolecules in solution, and won the IUCr Gjønnes Medal in Electron Crystallography along with Nigel Unwin (<http://www.iucr.org/news/newsletter/volume-25/number-2/chemistry-nobel-prize>).

More information about the Order of the Companions of Honour and Richard's career can be found at <https://www2.mrc-lmb.cam.ac.uk/richard-henderson-made-companion-of-honour/>.

AWARDS AND PRIZES

Sine Larsen awarded Tenth Max Perutz Prize of the ECA



The Tenth Max Perutz Prize of the European Crystallographic Association (ECA) has been awarded to Sine Larsen (University of Copenhagen, Denmark) in recognition of her multifaceted contributions to crystallography, including crystal structure analyses of organic molecules and proteins, charge-density studies and the development of synchrotron radiation facilities. Professor Larsen told the *IUCr Newsletter* that she was extremely happy and grateful to become a recipient of this Prize, adding "As my research has been in many areas of crystallography, I see it also as a recognition of crystallography as a multifaceted science."

Professor Larsen has served crystallographic science and related disciplines in important leadership roles, not least as IUCr General Secretary and Treasurer from 1993 to 2005, IUCr President from 2008 to 2011 and IUCr Immediate Past President until 2014. She was also one of the founding Main Editors of *IUCrj*.

Professor Larsen will receive the Prize at the Opening Ceremony of the [31st European Crystallographic Meeting](#) in Oviedo, Spain, on 22 August 2018, where she will present her Award Lecture.

Ada Yonath was the first to receive the Prize in 2000, followed by Jochen R. Schneider, Carmelo Giacovazzo, George Sheldrick, Eleanor J. Dodson, David Stuart, Claude Lecomte, Hartmut Füll, Randy J. Read, John Helliwell and Václav Petříček. More information can be found [here](#).

IUCR SUPPORTED EVENTS

IUCr supported meetings

These forthcoming meetings are supported by grants from the IUCr Calendar Committee.



**11th Oct 2026 - 16th
Oct 2026**
Indaba10

Skukuza, Kruger National
Park, South Africa



**5th Dec 2026 - 10th Dec
2026**
*African Materials Research
Society (AMRS 2026)*

Nairobi, Kenya

MEETINGS CALENDAR

Meetings calendar

This is a list of meetings of interest to crystallographers occurring within the next twelve months, as recorded in the IUCr Calendar of Events. Please let us know of any that are missing by [completing this form](#) or sending an email to forthcoming.meetings@iucr.org.

	Indaba10 South Africa 11th Oct 2026 - 16th Oct 2026
	Synchrotron Radiation: Science, Knowledge, Innovations, Future (SKIF-2026) Russian Federation 18th Oct 2026 - 23rd Oct 2026
	CCP-EM/Diamond Icknield Workshop United Kingdom 9th Nov 2026 - 13th Nov 2026
	Instruct-ERIC hands-on workshop on Advanced cryo-FIB-SEM methods Germany 9th Nov 2026 - 13th Nov 2026
	Crystal36-AXAA 2026 Meeting Australia 26th Nov 2026 - 2nd Dec 2026
	African Materials Research Society (AMRS 2026) Kenya 5th Dec 2026 - 10th Dec 2026
	Joint Polish-German Crystallographic Meeting 2027 Germany 15th Feb 2027 - 18th Feb 2027