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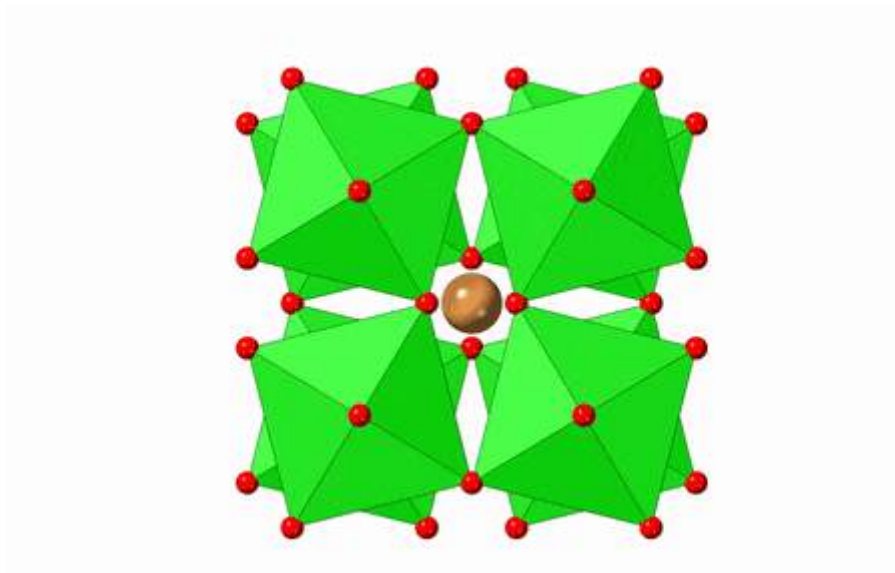
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EDITORIAL

The IUCr Newsletter goes from strength to strength

Mike Glazer



A tilted perovskite.

The initial launch of the new online *IUCr Newsletter* three months ago attracted a good deal of interest and we have been working hard to build upon this success. In this second issue you will note that we have a large number of articles of varied content. Topics covered include reports on meetings, developments in Africa, crystal growth competitions and other outreach activities. In addition, we have included a few articles of, I hope, general interest to crystallographers and others wanting to find out more about our subject. In particular, to get you thinking we have an unusual study of the symmetry of prime numbers as observed in terms of diffraction theory. My attention was drawn to this by a note on Twitter! I have also added an article myself on certain aspects of quartz crystals that you may not know, and we have in addition a fascinating idea related to early hominids and their observation of crystals, and how this might have influenced the development of early human intelligence. They seem to have been crystallographers at heart. Are we all here because of crystals?

As you will see, this issue includes some animations, something that could not be done before with the printed copy of the *Newsletter*. This I think adds more interest and makes our content eye-catching and at the same time informative. As I mentioned in the last *Newsletter*, I would like to have more submissions to include such dynamic content, *i.e.* films, animations, *etc.* I also would encourage our advertisers to make good use of this possibility.

I would welcome receiving your own articles of interest for future issues, and so at the bottom of each page you will find some buttons, one of which will enable you to [send in your own contributions](#) to the next *Newsletter* (March 2019). You can also submit material directly to any of our [Regional Editors](#) or directly to me at Newsletter.Editor@iucr.org. Such material should be submitted before 15 February 2019 to be considered for inclusion in the next issue.

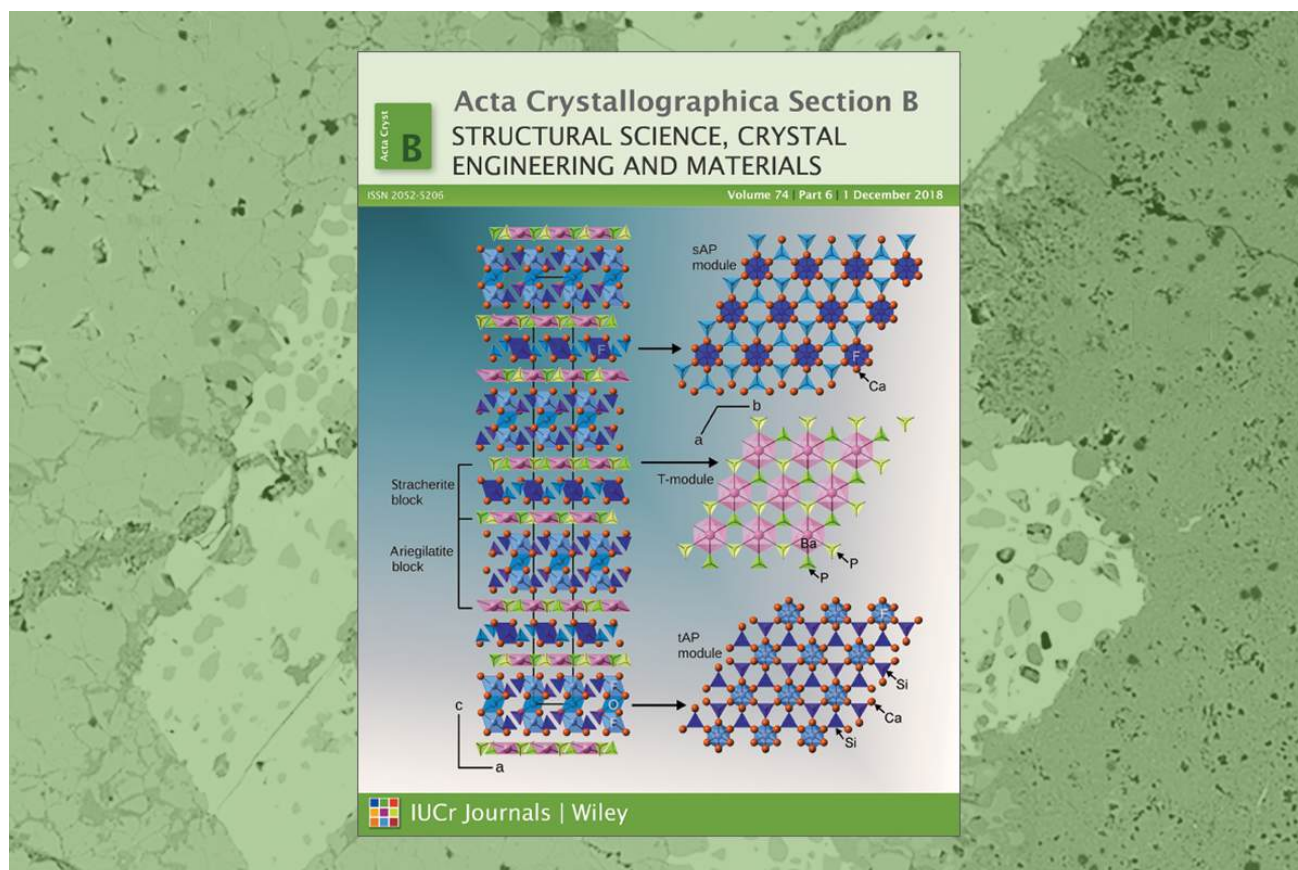
I am also keen to increase our mailing list (around 12,500 at present) to include other scientists and even members of the public who wish to be kept informed about crystallography and the work of the

International Union. You can help in this by drawing attention to our *News/etter* to others. To this end we have included a button to enable new readers to [sign up](#) for future issues. Note that it is planned that from 2019 onwards we shall have four issues per year.

I hope you enjoy this latest issue of the online *IUCr News/etter*. Do feel free to contact me at any time. I am happy to receive any comments, complaints (I hope not too many!) and suggestions for improvement or additions.

Acta Cryst. B: special issue on mineralogical crystallography

Sergey V. KrivovichevJanusz LipkowskiStuart J. Mills



For many centuries crystallography and mineralogy were part of a single discipline, and it was impossible to separate one from the other. In fact even the early works of Theophrastus (*On Stones*) and Pliny's *Natural History* show that the beginnings of both sciences have the same roots. In fact, crystallography grew out of mineralogy because in Steno's time the only crystals available for study were those of minerals. In the 20th century, however, the two sciences went their separate ways, but even today crystallographic research is an important part of mineralogy and mineralogical research is still an important part of crystallography. The [December 2018 issue of Acta Cryst. B](#) includes a special issue devoted to mineralogical crystallography and collects some important contributions that demonstrate the diversity of crystallographic ideas and methods developed to solve valuable issues in mineralogy.

There are some 5 500 (and growing) different mineral species known today [1] compared with more than 1 200 000 biological species described so far! Some of these mineral species are rare and occur in only a few localities, whereas others crystallize in the range of millions of tons in the Earth's crust. The latter are called 'rock-forming minerals' and their study is of utmost importance for our understanding of the behaviour of rocks on and beneath the Earth's surface.

Slightly less than 100 years ago, Vladimir Vernadsky wrote '... there is a close connection between the general chemistry studied in our events, which differs from the former not only in scale, but also in complexity' [2]. The unique character and richness of phenomena that we observe in the world of

mineralogical crystallography is definitely a consequence of the evolution of the mineral kingdom that involves many factors and trends that are not reproducible under laboratory conditions [3, 4]. The crystallographic studies of minerals are not only used to decipher the Earth's history but also have many applications in material sciences and technology. This is why we believe that the discipline of mineralogical crystallography is alive and will see considerably more advances in the near future. We are grateful to the authors of the papers of this issue for their interesting and important contributions.

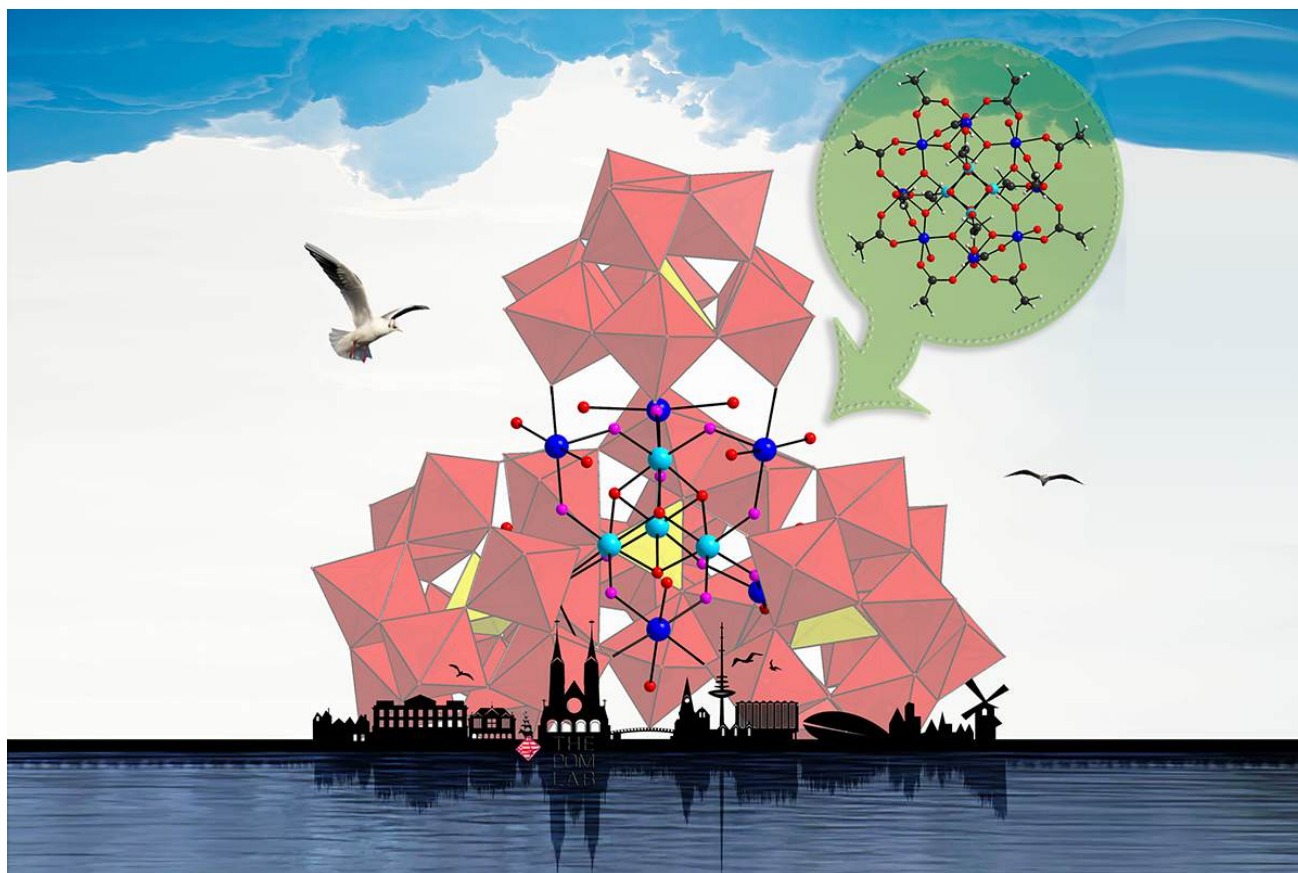
[1] Pasero, M. (2018). *The new IMA list of minerals*, accessed 4 December 2018.

[2] Vernadsky, V. I. (1923). *History of the Minerals of the Earth's Crust*. Petrograd: Nauchn. Khim.-Tekhn. Izd. (In Russian).

[3] Hazen, R. M., Papineau, D., Bleeker, W., Downs, R. T., Ferry, J., McCoy, T., Sverjensky, D. A. & Yang, H. (2008). *Am. Mineral.* **93**, 1693-1720.

[4] Grew, E. S., Hystad, G., Hazen, R. M., Krivovichev, S. V. & Gorelova, L. A. (2017). *Am. Mineral.* **102**, 1573-1587.

Acta Cryst. C: special issue on polyoxometalates



The [November 2018 issue of *Acta Crystallographica Section C Structural Chemistry*](#) marks a special anniversary of an exciting class of inorganic compounds: polyoxometalates (POMs). In their guest editorial, José Ramón Galán-Mascarós and Ulrich Kortz note that the very first POM structure, the so-called Keggin ion ($[\text{PW}_{12}\text{O}_{40}]^{3-}$), was structurally characterized by James F. Keggin 85 years ago in 1933 using powder X-ray diffraction. This was an important breakthrough for POM chemistry, as from then on structural aspects became more relevant and allowed the field to be developed more rationally. In the same year, Michael T. Pope was born, who went on to publish the book *Heteropoly and Isopoly Oxometalates* in 1983, widely agreed still to be the best introductory text to the field.

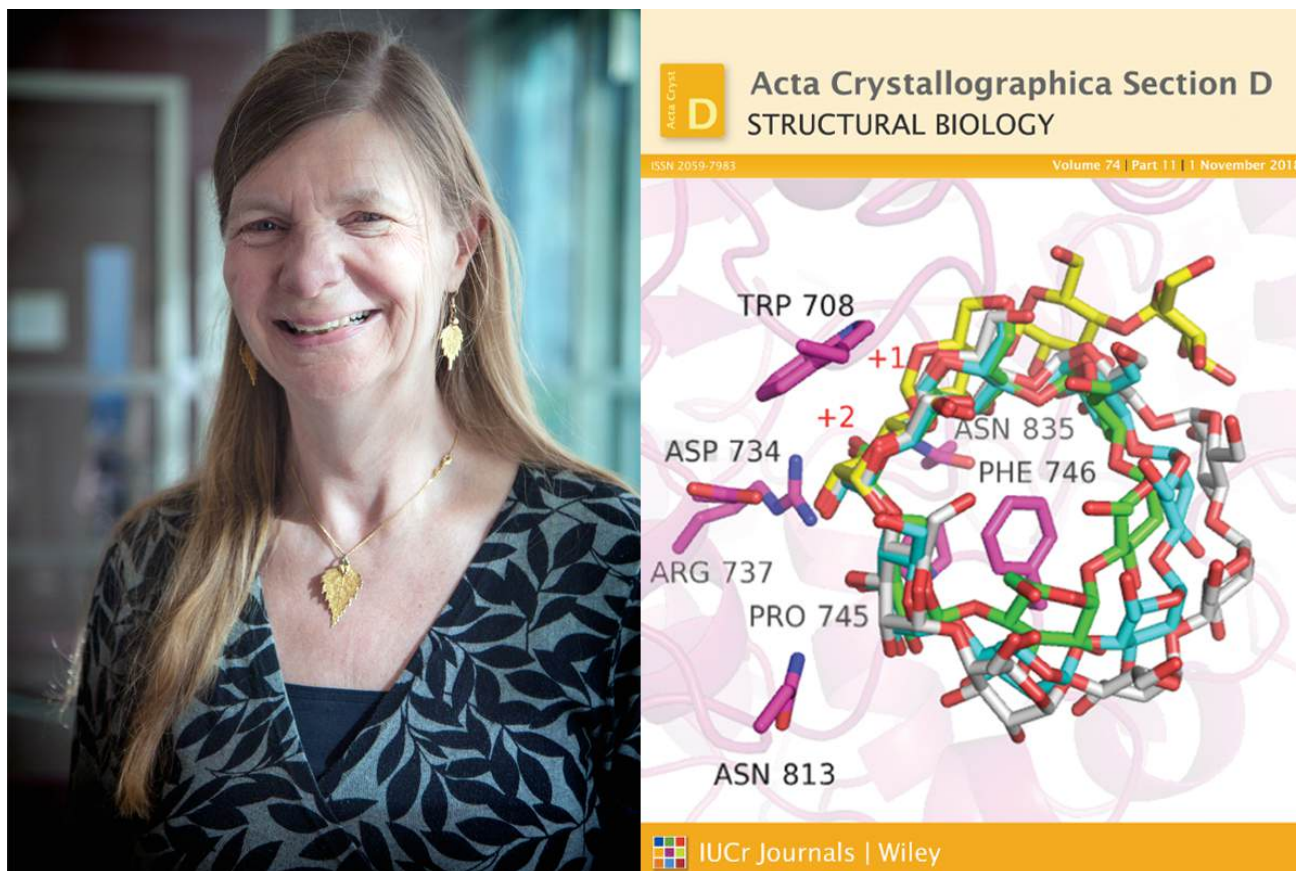
During the last half century or so, the development of POM chemistry has benefitted tremendously from single-crystal X-ray diffraction. Besides structural aspects, the study of the physicochemical properties of POMs has been developed tremendously in recent decades. The multitude of attractive properties includes controllable size, composition, charge density, redox potential, acid strength, high thermal stability in the solid state, solubility in polar/nonpolar solvents and reversible electron/proton storage. Such versatility renders POMs of interest for academic and industrial applications, especially in catalysis but also in fields such as medicine, magnetism, photochemistry and materials science.

It is also worth mentioning how POM chemistry has contributed to the development of crystallography itself. The presence of POMs (in particular heteropolytungstates) in solution often allows large biomolecules to be crystallized, and facilitates X-ray structure solution and refinement due to their high symmetry, robust molecular structure and heavy-atom content. The history of POMs has progressed from

the seminal work of Keggin (working under the supervision of Lawrence Bragg and influenced by Linus Pauling) developing powder X-ray diffraction analysis in the early 20th century, to the role of POMs as cocrystallizing agents for large biologically relevant molecules such as ribosomes, finally leading to the 2009 Nobel Prize in Chemistry (Ramakrishnan, Steitz and Yonath).

The contributions to this special issue on POMs provide an excellent overview of the current state of the subject, as well as providing updates to current research. *Acta C* is transforming from a structural (XRD) solid-state journal to a more general journal covering all aspects of structural chemistry, and the guest editors hope that this special issue on POMs will assist the journal in achieving its goals.

Elspeth Garman appointed as Section Editor of Acta Cryst. D



Elspeth is well known to many crystallographers and structural biologists, but for anyone who doesn't know who she is here is a brief summary.

Although she began her career as a physicist, Elspeth switched to the biological sciences in 1987 and is now Professor of Molecular Biophysics at the University of Oxford, UK. She is also Nicholas Kurti Senior Research Fellow in Macromolecular Crystallography, Brasenose College and was recently Director of the Systems Biology Programme at the Doctoral Training Centre, University of Oxford for five years, reflecting her interest in teaching as well as research. She is also a former President of the British Crystallographic Association and has won numerous awards.

Elspeth is one of the pioneers of research into radiation damage and cryoprotection of macromolecular crystals, and her work has had a major impact on structural biology. In 2008 she began her IUCr Journals career and was appointed as the Cryocrystallography Co-editor for the *Journal of Applied Crystallography*. For a number of years she has run workshops on radiation damage and guest edited the proceedings for the *Journal of Synchrotron Radiation*.

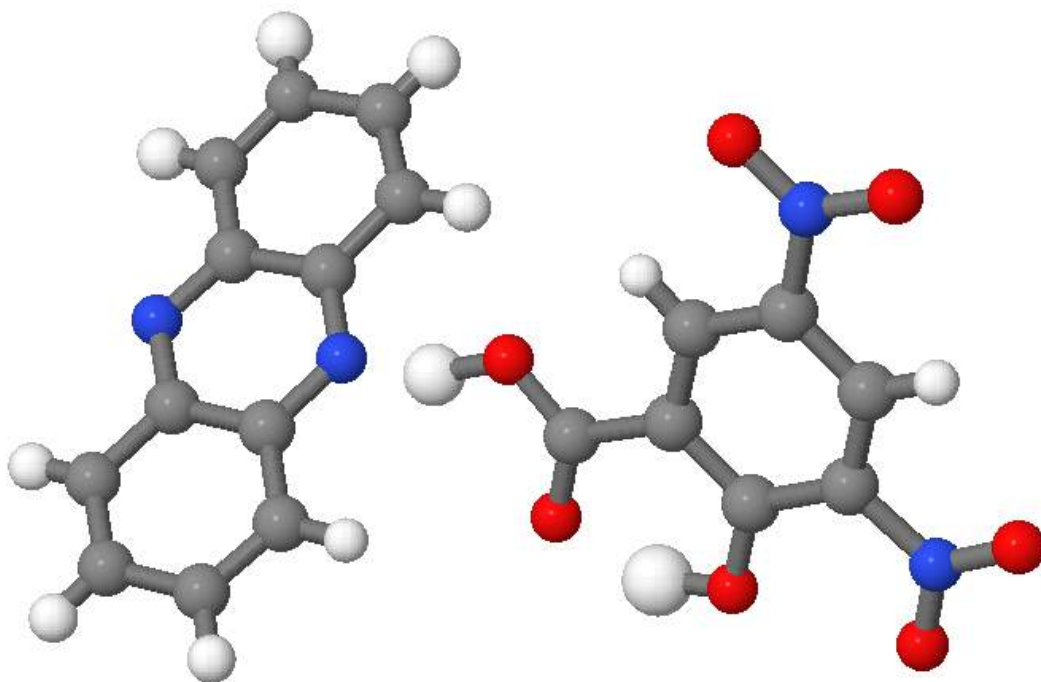
This is not the only area of crystallography where Elspeth has had an impact; she developed the proton-induced X-ray emission (PIXE) technique, which allows precise identification of trace metal elements within a protein structure, and has determined the structure of many proteins involved in infectious diseases. Her importance to structural biology was recognised in her appointment as a Co-editor for *Acta Cryst. D* (also in 2008), and she will continue to oversee the review of articles now that she is Section Editor.

It is in her role as a teacher and lecturer, however, that many of you may have come across Elspeth. She is a popular speaker and has an infectious enthusiasm for crystallography. She is involved in outreach programmes to increase public awareness and has appeared on many TV and radio programmes.

It is thus very exciting to welcome Elspeth to our editorial team and, to quote our other Section Editor Randy Read, we are 'absolutely delighted to be working with her!'.

RESEARCH NEWS

The importance of careful refinement



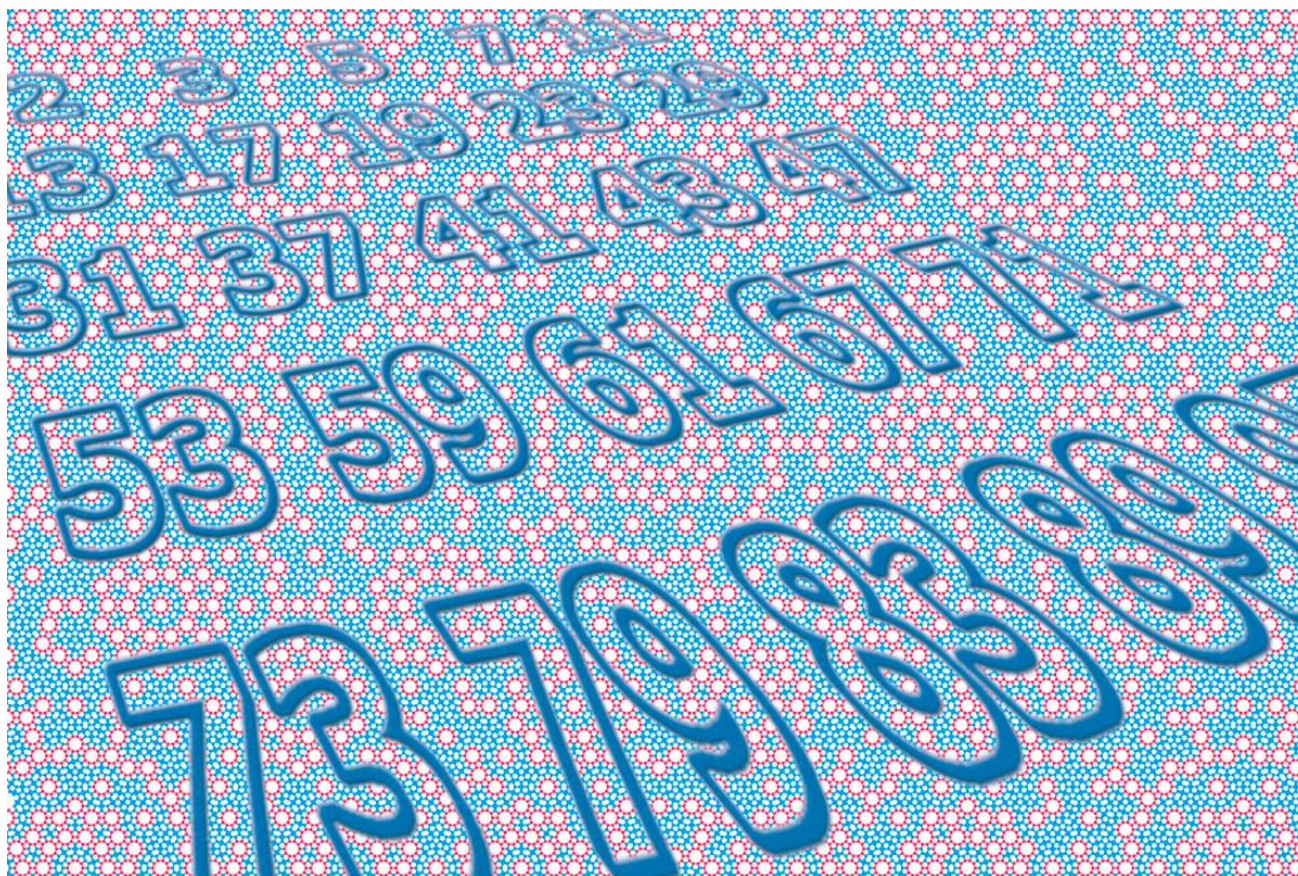
A large number of structural determinations of compounds containing 2-hydroxy-3,5-dinitrobenzoic acid and its various deprotonated forms, 2-hydroxy-3,5-dinitrobenzoate or 2-carboxy-4,6-dinitrophenolate, are biased. The reason for this follows from incorrectly applied constraints or restraints on the bridging hydrogen, which is involved in an intramolecular hydrogen bond between neighbouring carboxylic/carboxylate and oxo/hydroxy groups. This hydrogen bond belongs to the category of resonance-assisted hydrogen bonds. The position of the bridging hydrogen seems to be dependent on the pK_a (base), though with some exceptions. A stronger basicity enhances the probability of the presence of a phenolate. The problem of the location and refinement of such a bridging hydrogen, as well as that of the hydrogen atoms involved in the hydroxy group, and primary and secondary amine groups, is discussed in a recent article by Fábry [*Acta Cryst.* (2018). **E74**, 1344-1357]. It appears that the best model, in many cases, is obtained by fixing the hydrogen-atom positions found in a difference electron-density map while refining its isotropic displacement parameter.

"It is almost futile to state that modern automated diffractometers have enabled single-crystal X-ray structure analysis to become widely applied even by non-experts," commented Dr Fábry. "At the same time, however, it is important to emphasize that a large number of structure determinations of even simple molecules suffer from defects that are caused by inappropriately applied constraints or restraints. These defects bias not only the structure determinations themselves but also - more importantly - the overall information contained in the crystallographic databases. The present study of a whole family of the title molecules demonstrates the importance of careful refinement as well as of inspection of difference electron-density maps. I hope that this experience will reach especially those scientists for whom crystallography is not their specialization but nevertheless use it in their studies."

FEATURE ARTICLE

The building blocks of the integers

Gregory McColm



The prime numbers have a way of popping up in crystallographic conversations, and the recent results[i] on the structure factor of the primes by Matthew de Courcy-Ireland, Fausto Martelli, Salvatore Torquato and Ge Zhang should remind us of the role number theory plays in crystallography. Torquato, for instance, found that the structure factor for primes is characterized by dense Bragg peaks, like a quasicrystal, but positioned at certain rational wavenumbers, like a limit-periodic point pattern.

A positive integer is *prime* if it is divisible only by 1 and itself; thus 101 is prime because it is divisible only by 1 and itself, while 106 is not prime (it is called *composite*) as it is divisible by 53 as well as 1 and 106. The first 25 primes are 2, 3, 5, 7, 11, 13, 17, 19, 23, 29, 31, 37, 41, 43, 47, 53, 59, 61, 67, 71, 73, 79, 83, 89 and 97.

Prime numbers have been around a very long time, and the Greeks recognized that the primes were the basic building blocks of the integers. The Fundamental Theorem of Arithmetic says that every composite number is uniquely expressible as a product of powers of primes, and is thus divisible only by the primes in that product. For example, $1,860,824 = 2^3 \times 7^2 \times 47 \times 101$ is a product of only those prime powers and therefore is not divisible by any primes other than 2, 7, 47 and 101.

The fact that all positive integers are uniquely composed of prime powers, rather like species of molecules uniquely composed of atoms, has inspired much number theory. For example, if you try factoring large numbers on your pocket calculator you may notice that (1) primes are relatively rare among large numbers and (2) while a typical large number is composite, its largest prime factor is

relatively large. (In fact, in 1993, John Kemeny proved that if n is very large, about 69% of the integers between 1 and n have a prime factor larger than $\sqrt{n}$.)

But a diffraction result suggests that crystallographers might be interested in stepping back and looking at the distribution of primes among the integers. Euclid proved that there are infinitely many primes: if there was a largest prime p , then $p! = 1 \times 2 \times 3 \times 4 \times \dots \times p$ is divisible by every prime, so $p! + 1$ is not divisible by any prime, so since every composite number is a product of primes (by the Fundamental Theorem), $p! + 1$ must itself be prime, contradicting the claim that p is the largest prime.

And in a sense, primes seem to be everywhere. J. P. G. L. Dirichlet proved that if the greatest common divisor of positive integers a and b is 1, then there are infinitely many primes in the infinite set $\{a + bn: n = 0, 1, 2, 3, 4, \dots\}$. And as a consequence of the Prime Number Theorem - which I'll get to in a moment - for any real number $\epsilon > 0$, no matter how small, there exists a positive integer N such that if $p > N$ is prime, then the next prime q satisfies $q < (1 + \epsilon)p$: from a proportionate point of view, the gaps between successive primes shrink.

But while there are infinitely many primes, they seem to get increasingly sparser among larger and larger integers. For one thing, even if gaps between successive primes shrink in proportionate terms, in absolute terms there are larger and larger gaps between successive prime numbers: for any integer n , the integers $n! + 2, n! + 3, \dots, n! + n$ are all composite. And from a density point of view, the Prime Number Theorem of Jacques Hadamard and C. J. de la Vallée Poussin states that if the number of primes less than or equal to an integer n is $\pi(n)$, then for very large n , $\pi(n)$ is (proportionately) close to $n/\ln n$.

The distribution of primes seems to be rather irregular, but there are some regularities. For example, in 2004, Ben Green and Terence Tao proved that there are arbitrarily long arithmetic progressions in the primes. Nine years later, Yitang Zhang announced that for some integer $k < 70,000,000$, there are infinitely many pairs of primes p, q such that $q = p + k$. The bound on k has been improved substantially since then, and some mathematicians are optimistic that there will soon be an answer to the Twin Primes Problem: are there infinitely many pairs of primes that differ by 2 (such as 3 and 5, 11 and 13, 101 and 103, etc.)? Or are there only finitely many such pairs?

The Twin Primes Problem is a special case of a question that Zhang *et al.* were concerned with: given a k -tuple of integers $(0, a_2, a_3, \dots, a_k)$, with $a_2, a_3, \dots, a_k > 0$, do there exist infinitely many primes p such that $p, p + a_2, p + a_3, \dots, p + a_k$ are all prime? In fact, for a given usable k -tuple, are there enough such primes that they can be detected by diffraction (*i.e.* by a Fourier transform)? While this is impossible for some k -tuples [for any integer n , exactly one of $n, n + 2$, and $n + 4$ is divisible by 3, thus excluding $(0, 2, 4)$ as a usable 3-tuple], for other k -tuples they might even be common enough to be detectable by diffraction.

Primes show up almost everywhere in mathematics, and there are many open problems concerning them. "We don't understand primes very well," said Paul Erdős (who is also alleged to have said, "It will be another million years, at least, before we understand the primes"). On the other hand, John von Neumann said, "In mathematics you don't understand things. You just get used to them." That may make mathematicians like everybody else.

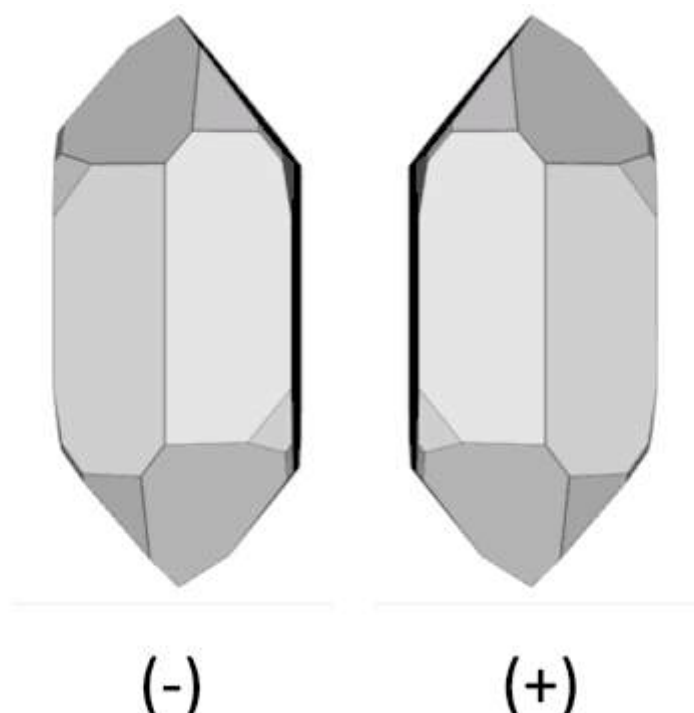
For further reading, one of the old warhorses of undergraduate number theory is Niven & Zuckerman's *Introduction to the Theory of Numbers*. The grand old book of number theory is probably Hardy & Wright's *An Introduction to the Theory of Numbers*. For computational applications, readers may be interested in Donald Knuth's *Art of Computer Programming*, volume 2: *Seminumerical Algorithms*, or the even broader *Concrete Mathematics* by Graham, Knuth and Patashnik. And Neil Sloane launched an [Online Encyclopedia of Integer Sequences](#), with information on many interesting sequences, from prime numbers to crystal coordination sequences.

[i] G. Zhang, F. Martelli & S. Torquato, *The structure factor of primes*, *J. Stat. Phys.* **A52**:11 (2018); S. Torquato, G. Zhang & M. de Courcy-Ireland, *Uncovering Multiscale Order in the Prime Numbers via Scattering*, posted on [ArXiv.org](https://arxiv.org); and S. Torquato, G. Zhang & M. de Courcy-Ireland, *Hidden Multiscale Order in the Primes*, posted on [ArXiv.org](https://arxiv.org).

FEATURE ARTICLE

Some musings on crystals of quartz

Mike Glazer



Try this. Go to Google and type in “crystals” and see what comes up. On looking for crystals of quartz I found the following:

This is the true ‘energiser’ crystal. Its clarity and simplicity are the keys to its power. It raises the vibration of the user and opens up the channels for healing and communication. When cloudy, it is believed to be a doorway to the mysteries. When clear, it is the power of Mother Earth herself. With Clear Quartz Crystal on or near you – you will experience an uplift of spiritual energy that imbues you with added strength and insight. As a healing crystal it works on all the chakras: balancing, clearing and energising. Clear Quartz Crystal has long been associated with mystics and magicians. Crystals and minerals remind us of the ‘elemental’ powers. In their solidity and bulk they appear unchanging and permanent. However, the real magic in them is that it is all an illusion and really they are constantly changing and evolving.

Clear Quartz Crystal is the true alchemist. Its transformation is a slow steady pulse in tune with the beat of Mother Earth. Those sensitive enough to attune can access the libraries within them. They all have a memory, some greater than others. It is about finding the right one for you.

Also, take a look at Gwyneth Paltrow’s website <https://goop.com/wellness/spirituality/the-8-essential-crystals/>. Now, I am sure that you will all have seen lots of pseudoscientific garbage like this.

Unfortunately, it is pervasive, and I have met several otherwise sensible, even well educated, people who nonetheless accept this nonsense. I have several times given talks about this other world of “pseudo-crystallography” to general audiences, only to find during question time that many still think there is something magical about crystals, that they emanate some sort of energy (they often use the quantum-mechanical term: energy levels!). I was even once threatened with violence by a man who phoned me to ask about the nature of crystals. The conversation started sensibly enough, but when I eventually said to him that crystals are the “deadest” objects in the universe, no energy emissions, no

auras, no chakras, nothing, nada, he turned nasty and, in the end, I reported the call to the police. People do not like having their cherished beliefs overturned. I think that we crystallographers need to speak out about such beliefs.

But I digress. I thought that it might be of interest to explain a few things about quartz crystals that you may not be aware of. It is one of my hobby-horses. I am sure you have all seen quartz crystals and so I have no need to describe them to you. They do look magical, but that is merely a consequence of their obvious symmetry coupled with a clear transparency. Such crystals are also known as rock crystal. Now the crystal structure of quartz has been well documented for around 80 years and you would have thought that there can be little more to say about it. But you would be wrong! Quartz crystals are extremely complex, especially regarding their habit and varieties of twinning. A good website to learn about the complexities of quartz crystals is <http://www.quartzpage.de/intro.html>. Synthetic quartz crystal is a strategic material with particular applications in frequency control (more on this later) with a global annual market value of around USD 72 million in 2017, projected to grow to around USD 95 million by 2022.

The first point to note is that from a crystallographic point of view the majority of structure descriptions in the literature are in fact incorrect. The first problem arises because quartz crystallizes in one of two possible space group types, $P3_121$ and its enantiomorph $P3_221$ (so-called left and right crystals, respectively). Furthermore, there are two possible orientations, known as obverse and reverse, when viewed perpendicular to the c axis. This makes for four possible arrangements. To complicate things even more, we crystallographers normally refer to crystal structures using a right-handed coordinate system, whereas crystal growers, using the crystal morphology as a criterion, refer to right and left crystals using axes of opposite hand! So that now gives us eight possible descriptions. Does this matter? Well it does if you want to order a slice of quartz in a particular orientation from a supplier: be aware that you may not get the actual cut you wanted.

Recently I purchased a rather nice quartz crystal (Figure 1), which I bought from a market stall in the town of Banbury (UK). Of course, the market stall-holder was selling her crystals as magical healers. But I managed to hide my distaste at being promised that it would bring harmony to me, as the crystal was especially beautiful! In fact, I was particularly attracted to the fact that this crystal possessed a small rectangular face (highlighted in the figure), which is a characteristic indicator of the so-called hand of the quartz crystal. You don't see this so clearly in most natural quartz crystals that I have seen. So what is its significance?



Figure 1. The quartz crystal purchased by the author.

As far back as 1978, Donnay and Le Page[i] wrote the definitive paper on this problem, entitled “On the vicissitudes of the settings of quartz”, which gave a complete set of explanations and recommendations. However, despite this, errors continued to occur. Because of this I recently felt obliged to add my own contribution to the discussion by writing up a simple description in a recent paper[ii] that I dedicated to the late Helen Megaw, who had tried hard herself to get the structural description right, but in the end she too had failed.

To understand this, a few years ago, 1811 to be precise, Dominique François Jean Arago (1786-1853), in France, observed that colour developed in plates of rock crystal when polarized light was transmitted through them in a particular direction. This was the first observation of the phenomenon that we now call optical rotation. Pretty soon this effect was observed in solutions of various organic molecules and Jean-Baptiste Biot (1774-1862), again in France, realized that this must be a property inherent in the molecules themselves: *Cette propriété consiste dans la faculté qu’ont les molécules dont il s’agit de faire tourner d’un certain angle, et dans un certain sens les axes de polarization de rayons lumineux*. Such was the intense scientific interest in this phenomenon that by 1820 most of the fundamental experiments needed to understand optical rotation had already been realized. Now, earlier, René-Just Haüy (1743-1822), yet again in France, observed that certain quartz crystals, to which he assigned the name “Plagièdre”, showed unsymmetrical faces, although he thought it was a random phenomenon. Biot

also discovered that, on the basis of the unsymmetrical faces, crystals of quartz could be separated into two sorts that were of opposite hand and that they rotated polarized light in opposite directions. The figure at the top of the page shows idealized drawings of left and right crystals of quartz. In 1820, the physicist Frederick William Herschel (1738-1822) working in England – yes, the famous astronomer who discovered the planet Uranus – sorted some quartz crystals in his possession depending on the direction in which the unsymmetrical faces leaned. He then arranged for each crystal to be sliced and polished and, like Biot, observed that polarized light rotated in opposite directions for the two forms. He was then able to link the sense of rotation of polarized light to the actual crystal faces, writing thus *“Quartz samples whose hemihedral facets point in the same direction rotate the polarized light in that direction: a right hemihedral produces right rotation – and vice versa”*.

Some years later, in 1848, Louis Pasteur (1822-1895), in France once again, reported on his famous experiment showing that sodium ammonium tartrate crystals could be divided into portions that were mirror images of each other on the basis of their morphology, and more importantly this conferred a corresponding change in the sense of rotation of polarized light when the crystals were dissolved in water[[iii](#)]. Personally, I consider this to be his greatest scientific discovery, because later around 1860 Pasteur was led to the view that, as solutions of biological organic compounds also showed optical rotation, chirality or handedness (he called it dissymétrie) was an essential component of nature. It took nearly another 100 years for Crick and Watson to prove the point. So much for our funding agencies who seem to think that scientific impact can be so easily predicted!

Finally, do you know why we use quartz crystals in our watches? The first point to understand is that quartz is a piezoelectric material. The piezoelectric effect, where application of an external stress creates an electric polarization, was discovered in 1880 by the brothers Jacques (1856-1941) and Pierre Curie (1859-1906) (France again!). In the so-called converse piezoelectric effect, discovered in 1881 by Jonas Ferdinand Gabriel Lippmann (1845-1911) (France!), application of an electric field causes a strain deformation to be set up in the crystal. Therefore, in simple terms, application of an oscillating electric field makes the crystal change shape in an oscillatory fashion. A slice of quartz crystal can then be made to exhibit resonance depending on the frequency of the electric field, the particular cut section and its thickness. It is worth noting that up to and including World War 2, the piezoelectric resonance of quartz working at about 50 kHz was used to send out underwater ultrasonic signals (by the converse effect) to bounce off enemy submarines and then detect the returning signals (by the direct effect). This was originally called ASDIC in the UK, and those employed in designing the equipment for this were not allowed for security reasons to mention the word “quartz”: instead they were supposed to call it “asdivite”! Later the USA changed the name to SONAR, which is the way we refer to it today. Quartz is no longer the material of choice in this application, as there are more strongly piezoelectric substances available that can function at a more useful lower frequency of about 5 kHz. Anyway, what about my quartz crystal: is it left or right? Well, I had observed the unsymmetrical face (marked *s* in Figure 2) when I bought the crystal, and the way it is tilted suggests that it is a right crystal, *i.e.* that when viewed down the *Z* axis polarized light would rotate clockwise as viewed by an observer[[iv](#)]. It would have been more definitive if the crystal also showed the more obvious unsymmetrical face marked *x* in Figure 2, but there you go: you can’t have everything! I haven’t had the heart to have it sliced up to prove it. However, it is rare for quartz crystals to show all the faces of an ideal crystal (Figure 2). In addition to the face marked *s*, there are three large faces marked *R* and three small ones marked *r*. In my crystal, however, *R* and *r* are approximately the same size and so I can only rely on face *s* to determine the optical hand. Do look out for these indicator faces when you next see a quartz crystal.

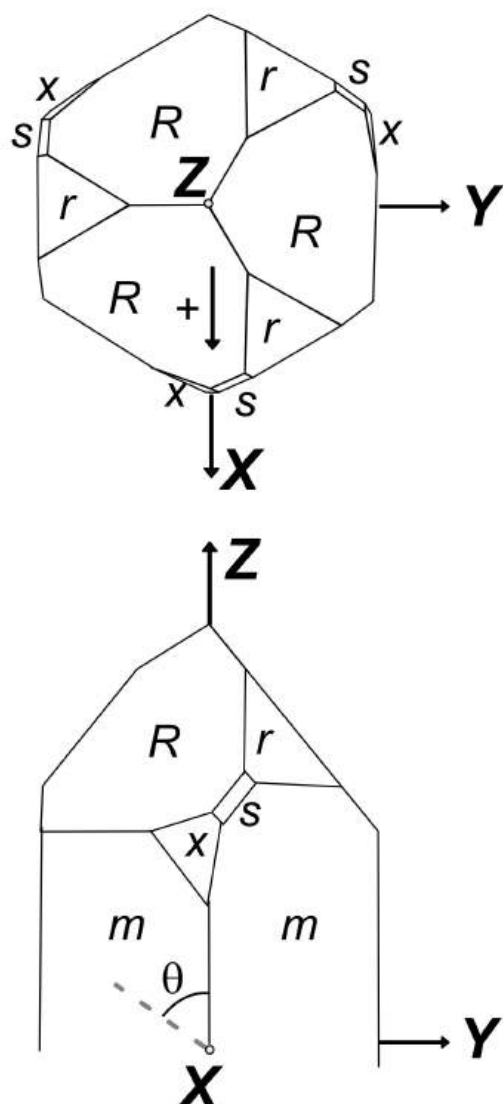


Figure 2. Right (dextro) handed quartz.

Returning to timekeeping, the resonance frequency is used to control the watch's time. In watches a frequency of 32.768 kHz is normal. However, quartz is not a particularly strong piezoelectric: there are many other materials that are more piezoelectric. However, it does have a special, and almost unique, property that is important for accurate timekeeping. To understand this, consider the formula for frequency in terms of the elastic stiffness coefficient c , the density ρ and the crystal thickness l ,

$$f = \frac{1}{l} \sqrt{\frac{c}{\rho}} \quad (1.1)$$

and then the temperature coefficient of frequency has the form

$$\frac{1}{f} \frac{df}{dT} = \frac{1}{2c} \frac{dc}{dT} - \frac{1}{l} \frac{dl}{dT} - \frac{1}{2\rho} \frac{d\rho}{dT} \quad (1.2)$$

Now, the second term is the linear thermal expansion coefficient α with a value of around 10^{-5}K^{-1} , and the third term is proportional to α (for an isotropic solid it is 3α). Both are generally positive quantities as

bonds become weaker with increasing length during rising temperature. But it is possible, in principle, that the first term, the temperature coefficient of stiffness, could cancel with the other two terms. The following table shows some examples of the temperature coefficients of the elastic stiffness for some oxides.

Table 1. Temperature coefficients of elastic stiffness in units of 10^{-4}K^{-1}

MgO	$T_{c_{11}} = -2.3$	$T_{c_{44}} = -1.0$
SrTiO ₃	$T_{c_{11}} = -2.6$	$T_{c_{44}} = -1.1$
Quartz	$T_{c_{11}} = -0.5$	$T_{c_{33}} = -2.1$
	$T_{c_{44}} = -1.6$	$T_{c_{66}} = +1.6$

From this you can see that most coefficients are negative reflecting the fact that the crystals become softer with heating. But note that in quartz, one of the shear elastic stiffness coefficients $T_{c_{66}}$ is actually positive. This then makes it possible for Equation (1.2) to equal zero and so, provided that the correct section of quartz is cut, the frequency can be temperature-compensated. After all, you don't want your watch time to change when you move from a hot to a cold place! This is the main reason why quartz, rather than other piezoelectrics, is used in watches and in high-end frequency-control systems[v].

Now what is the origin of this anomalous increase in shear stiffness in quartz? The clue is in considering the change in crystal structure with temperature. At room temperature the space group is $P3_121$ for right-dextro quartz (or $P3_21$ for left-laevo quartz) and has distorted sixfold rings of Si-O units about the 3_2 -fold axis at the unit cell origin. These rings are floppy. At about 846 K, there is a phase transition to a structure in space group $P6_222$ (or $P6_422$): in this case the 3_2 axis at the unit-cell origin becomes 6_2 , and so the Si-O groups occur in perfect 6_2 -fold rings and are then locked in place (Figure 3).

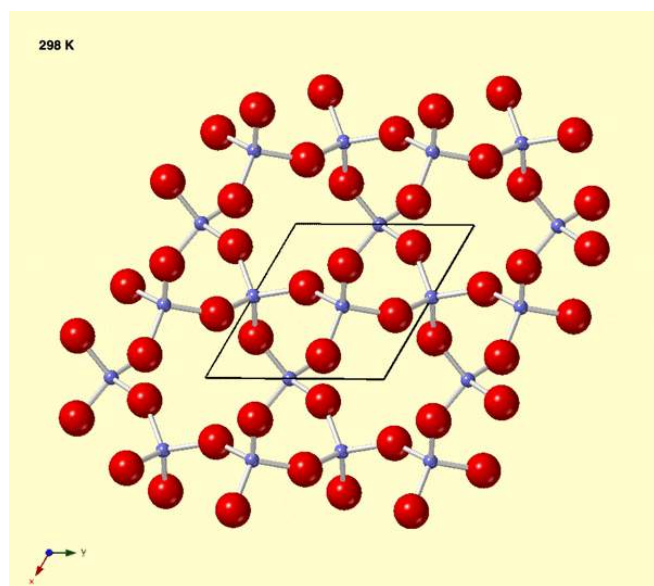


Figure 3. Transformation from low- to high-temperature quartz structure. Image created with *CrystalMaker X*.

So on heating from room temperature the structure tends to become stiffer against shear about the Z axis with respect to the Si-O rings. However, to achieve this temperature compensation it is necessary to select a particular cut of the crystal, and this has to be done to within a tiny fraction of a degree. The usual section is known as the AT cut and is at $\theta = 35^\circ 25'$ (Figure 2). The website <http://www.roditi.com/>

[SingleCrystal/Quartz/QuartzHead.htm](#) is well worth reading as it gives details on how crystals of quartz are grown and cut for frequency applications. Crystals are sliced into bars and then oriented using X-ray diffraction before being cut into the required slices. Because of the difficulty of getting the perfect cut angle, the slices are then tested for their different qualities and temperature stability and then binned according to the results, with the most expensive being those that are closest to ideal behaviour.

Having said all this, you might think that your cheap Mickey Mouse watch would be less precise than your expensive Omega. But you would be wrong. The evidence is that both can keep time to within roughly the same precision, partly because the typical temperature variations in practice are relatively small. However, in the frequency control market for electronics, military and communications industries very precise temperature compensation does matter a lot.

Let me finish with an anecdote from W. L. Bragg. I am grateful to John Helliwell for reminding me of this story:

"We were staying in Ballater, a small town on Deeside in Scotland. In the town was a tiny shop which sold tourist attractions and picture postcards, and in its minute window was a very fine specimen of smoky quartz mineral. Buying a postcard, I said to the proprietor, 'That's a fine group of smoky quartz in your window' and had this reply in very broad Scotch: 'That's no smoky quartz, that's topaz. It's a crystal. You can tell crystals by the angles between their faces. If you're interested I'll lend you a book on the subject.' I knew enough (crystals being rather in my line) to be sure it was smoky quartz and on return to base looked up a book on Mineralogy which said 'Smoky Quartz, also known as Cairngorm, is called Topaz in Scotland.'"

[i] Donnay, J. D. H. & Le Page, Y. (1978). *On the vicissitudes of the settings of quartz*. *Acta Cryst.* **A34**, 584-594.

[ii] Glazer, A. M. (2018). *Confusion over the description of the quartz structure yet again*. *J. Appl. Cryst.* **51**, 915-918.

[iii] An excellent detailed review of Pasteur's work on crystals is given by Flack, H.D. (2009). *Louis Pasteur's discovery of molecular chirality and spontaneous resolution in 1848, together with a complete review of his crystallographic and chemical work*. *Acta Cryst.* **A65**, 371-389.

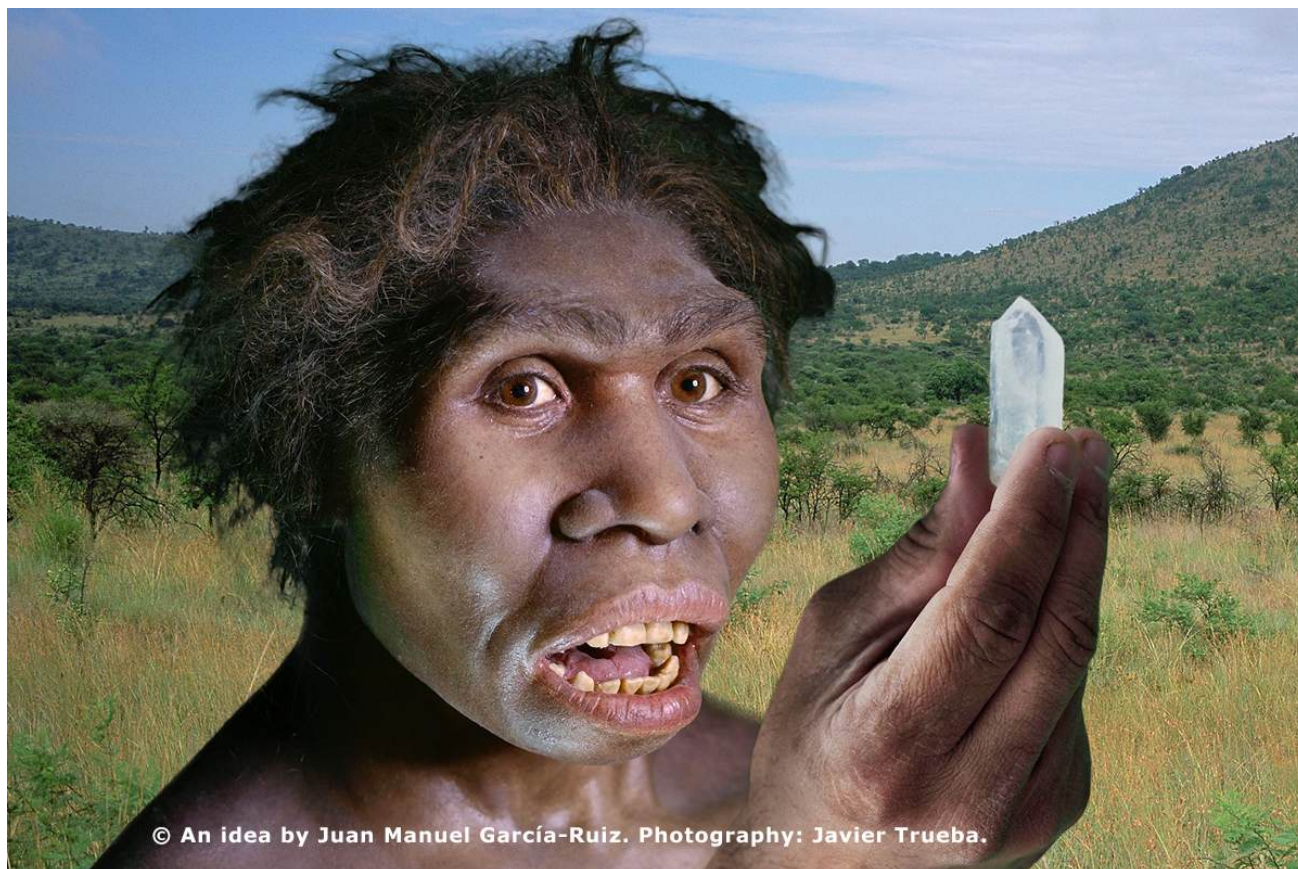
[iv] By the way, we know that the sense of rotation correlates with the helical arrangement of Si-O groups around the 3_1 (or 3_2) axes of symmetry at $1/3$, $2/3$, z for laevo (or dextro) quartz. This has caused confusion in the past because when we talk about rotation of polarized light we consider the light coming towards the viewer, but when we refer to a helical arrangement in the crystal structure the convention is to define the sense of the helices away from the viewer. Thus, in right (dextro) crystals of quartz the corresponding helices around the 3_2 axes are left-handed!

[v] You can read more about this in a 1973 article by R. E. Newnham at <http://www.dtic.mil/dtic/tr/fulltext/u2/760766.pdf>.

INTERVIEW

Wrestling with questions at the edge of science methods

John R. Helliwell



Recently, Professor Juan Manuel García-Ruiz published a delightful, well written essay [1] on the mysteries of what catalysed thinking, symbolism and consciousness. Surely a very important topic. But how to approach it? He does so by posing this question in the context of pre-evolution, and then evolution, of hominids admiring the straightness of crystal edges of the abundant quartz. In reading his essay I subsequently communicated with him by email, following my complimentary preamble above:

JRH: JuanMa, quartz is the second most abundant crystal on Earth behind feldspar (see <https://en.m.wikipedia.org/wiki/Quartz> and <https://en.m.wikipedia.org/wiki/Feldspar>). So I am wondering why the second most abundant crystal would have such an influence, rather than feldspar.

JM: Thank you very much for your interest and comments. Certainly, feldspar is more abundant than quartz, but it rarely appears as isolated single crystals as quartz does. Feldspar is a rock-forming mineral that in most cases appears as micro or macro (pheno)crystals with other minerals. Therefore, it is difficult to observe them as three-dimensional isolated objects. However, quartz appears in many outcrops as single crystals in sedimentary environments (Spanish jacinto, or the New York "diamonds") but also in igneous rocks as large crystals in geodes and druses.

JRH: Also might calcite and its delightful double refraction optical effect (<https://en.m.wikipedia.org/wiki/Birefringence>) allow a further elaboration of the theory?

JM: Calcite is a very singular case. Calcite crystals are not described in the oldest lapidarium and curiously the phenomenon of double diffraction was unknown until the XVI or XVII century. There is no proof, for example, of the use of calcite by the Vikings.

JRH: Finally, just to mention also that I recall your delightful lecture on this whole topic at an American Crystallographic Association conference.

So, I commend this thought-provoking essay to you, the reader.

Editor's comment

JuanMa's *Substantia* article makes some interesting observations relating how ancient hominids viewed the world around them and how the discovery of quartz crystals in particular may have been the cause of advances in thinking. He points out that the world of these early humans was one in which everything visible around them was dominated by curves and irregularities. But the quartz crystal was probably the only object that they saw that had straight edges. JuanMa mentions that unmodified crystals of quartz have been found to be associated with ancient hominid sites, suggesting that these people collected the crystals for their aesthetic value rather than for utilitarian purposes. Here he points to an analogy with the famous film "2001: A Space Odyssey" in which a mysterious black perfect slab is discovered planted on earth, presumably by an alien civilisation, and this sparks off the imagination of the primitive creatures that discovered it. JuanMa explains that the black slab was actually intended to be a crystal but that it was coloured black for filming purposes. So, an interesting question arises: suppose that crystals were not discovered by ancient hominids: would this have stalled intellectual development?

[1] J.M. García Ruiz (2018). <https://doi.org/10.13128/Substantia-57>

AWARDS AND PRIZES

Call for nominations for the twelfth Ewald Prize



It's that time of the triennium when the IUCr invites your nominations for the Ewald Prize for outstanding contributions to the science of crystallography. The Prize is named after Paul P. Ewald, in recognition of his significant contributions to the foundations of crystallography and to the founding of the IUCr. Professor Ewald was the President of the Provisional International Crystallographic Committee from 1946 to 1948, the first editor of the IUCr publication *Acta Crystallographica* from 1948 to 1959 and the President of the IUCr from 1960 to 1963.

The Prize is presented once every three years during the triennial International Congresses of Crystallography and consists of a medal, a certificate and a financial award. The recipients to date are as follows:

Year	Place	Recipients
1987	Perth, Australia	Professor J. M. Cowley and Dr A. F. Moodie
1990	Bordeaux, France	Professor B. K. Vainshtein
1993	Beijing, China	Professor N. Kato
1996	Seattle, WA, USA	Professor M. G. Rossmann
1999	Glasgow, UK	Professor G. N. Ramachandran
2002	Geneva, Switzerland	Professor M. M. Woolfson
2005	Florence, Italy	Professor P. Coppens

Year	Place	Recipients
2008	Osaka, Japan	Dr D. Sayre
2011	Madrid, Spain	Professor E. Dodson, Professor C. Giacovazzo and Professor G. M. Sheldrick
2014	Montreal, Canada	Professor A. Janner and Professor T. W. J. M. Janssen
2017	Hyderabad, India	Professor T. L. Blundell

The twelfth Prize, for which nominations are now being invited, will be presented at the [Prague Congress](#) in August 2020.

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

Nominations for the Ewald Prize should be submitted electronically using the [Ewald Prize Nomination Form](#) to the IUCr Executive Secretary at execsec@iucr.org. The closing date for nominations is **31 August 2019**.

AWARDS AND PRIZES

Call for nominations for the 2020 Gjønnnes Medal in Electron Crystallography



2017 Gjønnnes Medal winners Richard Henderson (left) and Nigel Unwin with incoming CEC Chair Louisa Meshi.

The Gjønnnes Medal in Electron Crystallography is awarded every three years and recognizes an outstanding contribution to the field of electron crystallography. The Gjønnnes Medal is accompanied by a certificate and funding to present an invited Keynote Lecture at the triennial International Congress of Crystallography.

Administration

This award is managed by the Awards Sub-committee of the [Commission on Electron Crystallography](#) (CEC) of the IUCr. This Sub-committee is responsible for soliciting and evaluating and recommending a nominee to members of the CEC for final approval, or recommending that no award be made.

Rules and eligibility

Nomination for the Gjønnnes Medal is open to scientists and engineers in all areas of electron crystallography defined in the broadest context as the branch of science that uses electron scattering and imaging to study the structure of matter. Nominees of any nationality are eligible. It is expected that the nomination will be for a single person. However, since breakthrough innovations often involve more than one individual, the nomination can be for two or three people, maximum. In the case of multiple nominees, it must be shown that each person contributed roughly equally to the innovation.

The Award will not be bestowed *in absentia* except in extraordinary circumstances. Current members of the CEC, members of the IUCr Executive Committee and previous recipients of the Gjønnnes Medal are not eligible.

Nomination procedure

Nominations are invited for the next Gjønnnes Medal, which will be awarded at the [IUCr Congress in Prague, Czech Republic](#), in August 2020.

The nomination packet should be sent to the Chair of the CEC, Professor Louisa Meshi (louisa@bgu.ac.il), and should include the following:

- A letter of not more than 3000 characters evaluating the nominee's qualifications in the field of electron crystallography and identifying the specific work to be recognized. There is no nomination form, so this letter is considered the nomination 'application'.
- *Curriculum vitae* of the nominee.
- A list of the most important publications of the nominee.
- At least two, but no more than four, seconding letters.

The deadline for receipt of nominations is 30 April 2019.

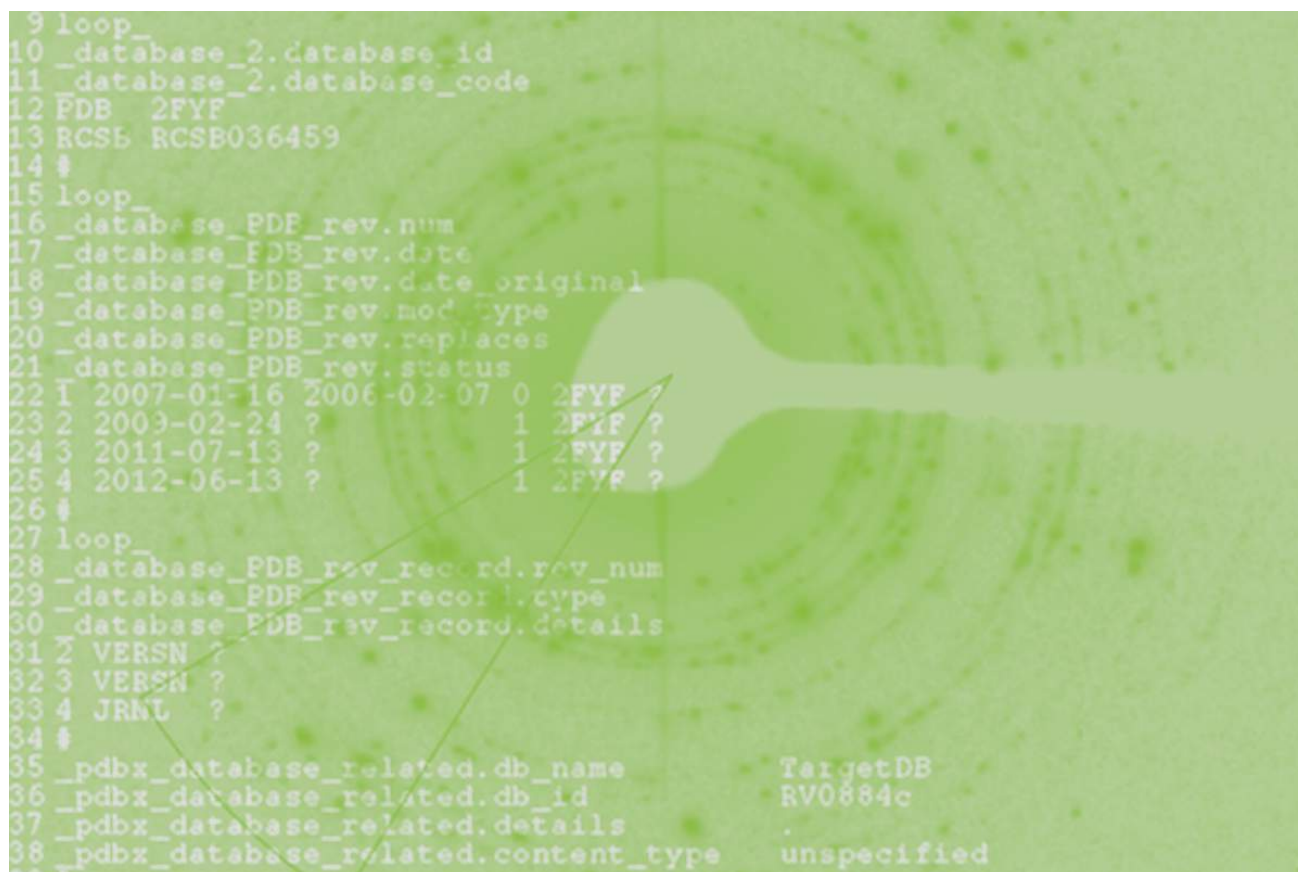
Previous recipients

[Previous recipients](#) have included the Nobel Prize winner Richard Henderson, who along with Nigel Unwin, received the 2017 Gjønnnes Medal at the 24th IUCr Congress in Hyderabad, India, for the development and powerful application of structural determination methods for biological complexes at near-atomic resolution using electron crystallography. In 2014, John Steeds and Michiyoshi Tanaka were awarded the medal for their outstanding contributions to convergent-beam electron diffraction, and the 2011 awardees were Archie Howie and Michael Whelan for the development of the dynamical theory of diffraction contrast of electron microscope images of defects in crystals, and other major pioneering contributions to the development and application of electron microscopy, diffraction and spectroscopy of materials. The medal is named in honour of its first recipient, Jon Gjønnnes, who received the award at the 21st IUCr Congress in Osaka, Japan, in 2008. He said "The basic scientific achievements of the last century - which one may epitomize by three words: the atom, the computer and the gene - rest on two main efforts: Quantum theory - which is prerequisite to our understanding of the atoms and the way they are put together, Crystallography - which is the basic, never-ending task of exploring the atomic architecture of matter".

IUCR ACTIVITIES

Reasons for raw data archiving and reuse in chemical crystallography

Simon Coles Amy Sarjeant, with a Foreword by John R. Helliwell



Foreword

Crystallographers have a long-standing tradition of linking the underpinning data to their publications. Chemical crystallography has led the way, harnessing new technologies for data storage as well as carefully defining its metadata via the world-renowned crystallographic information file (CIF) and developing an extensive [checkCIF](#) procedure for vetting these data. *Acta Cryst. C* has also led the way with its exemplary article submission procedure comprising the authors' narrative, their underpinning coordinates and structure factors along with the *checkCIF* report. Thus an editor and referees can undertake direct calculations and scrutinise the outcomes (alerts) highlighted in the standardised *checkCIF* process. Readers thereby enjoy articles with data carefully vetted at the highest degree possible and the databases likewise can then harvest these perfect fruit. In recent years there has been a major increase in digital storage capability along with an expansion of generic data archives such as those provided by individual universities or administered centrally such as the EU's Zenodo. Naturally the question has now arisen as to the need for the preservation of raw i.e. experimental diffraction data sets, and across all of crystallography. That it is feasible and that it is recommended was the top recommendation of the IUCr's Diffraction Data Deposition Working Group (DDDWG) in their [final report](#) presented to the IUCr in 2017 in Hyderabad. This would also continue to keep the IUCr in line with the general exhortation for scientific data to be FAIR, i.e. Findable, Accessible, Interoperable and Reusable. The individual IUCr Commissions are now digesting the IUCr DDDWG Final Report. The DDDWG has been

incorporated into the IUCr's new Committee on Data (CommDat). Two members of CommDat, Amy Sarjeant and Simon Coles, communicate with the structural chemistry community now via a questionnaire.

I encourage you to take part in providing your answers to the questionnaire.

Thank you.

John R. Helliwell

Chair of IUCr CommDat and Chair of the IUCr DDDWG (2011-2017).

It is now common to deposit structure factors when publishing journal articles and this now caters very well for routine small-molecule structures. However, this is only the case if everything in a raw image is fully and/or properly accounted for and the model is correct or appropriate. In some cases raw data may no longer be required, but in others it may be necessary to validate or 'do better' in the future. Now is the time to explore raw data archival practice and gather opinions as to if/how raw data could/should be used if it were to be made more widely available.

'Data' can generally be considered to be raw data, processed data and derived data - in the crystallographic context these are namely diffraction images, structure factors and crystal structures, respectively. Recently some progress has been made in that software will include derived data (structure factors) in the CIF result and that validation processes and the Cambridge Structural Database (CSD) will make use of and curate this data. But we can go further still - not only could raw data improve validation processes and provide valuable training sets for software developers to improve algorithms, etc., but there is a more interesting issue. A diffraction experiment records the average signal from the whole sample, which includes defects, impurities, etc., yet often only the data to get a perfect result is extracted. For materials engineering it can be crucial to be able to understand these additional effects, yet it is never made public that they have been observed!

Raw data availability therefore can be very important; however, there are often further counter arguments around the overhead to doing this. The diffraction experiment is relatively quick and cheap, so why not just do it again? The real cost of doing a structure again was assessed by the UK National Crystallography Service as part of the 'Keeping Research Data Safe Project'. There are many nuances to such a costing, but if one has to factor in that the research expertise/group/laboratory that originally generated the material may not exist any more or may not still be specifically set up (people, apparatus, etc.) to make such materials, then the cost rapidly escalates. The replacement cost of the CSD is therefore almost unmeasurable!

Barriers to raw data archival include file size, file format interoperability, and a lack of perceived need. The macromolecular community has recognized the need for raw data archival and various workflows and deposition standards have arisen to meet this need. However, the small-molecule community lags behind.

Data transfer and storage problems are now being overcome and for around 15 years there has been an 'extension' to CIF (*imgCIF*) that can cater for raw data, yet its uptake by the small-molecule community has been very slow indeed. So why aren't we amassing more of our valuable raw data for the community to widely exploit? For the last five years a group, known as the Diffraction Data Deposition Working Group, has been looking into the issues surrounding this topic. The outcome from the activity of this group is that the IUCr has recently convened a Committee on Data, 'CommDat' as an advisory committee to the Executive.

It is generally assumed that small-molecule crystallographers do archive raw data, but that it is not archived in the 'best' way, i.e. easily searchable, in a 'structured' environment and that this community

does not think about making raw data visible outside of their own use. We are therefore looking to find out the following:

- The extent to which small-molecule crystallographers archive raw data (in a sharable way?) and what stands in their way.
- How much 'educating' of crystallographers is required to illustrate the benefits of archiving (both for oneself and for others).
- How could raw data archives be used in validation, e.g. would it be more justifiable to publish a 'poorer' result if raw data were made available?
- What are the driver(s) for the community in terms of using the contents of a raw data archive.

We have created a survey to canvass the small-molecule community to determine the answers to these questions. Whether you currently actively archive your raw data or not, we encourage you to take part in order to help to better define the problems and barriers to this important endeavour. The survey explores the following two themes:

1. Your archived raw data: why? where? managed? searchable? available? ever revisited?
2. Different people in different roles might have different drivers/reasons for archiving and revisiting raw data. We suggest the following as some food for thought and want to canvas views around these and any other related matters:

- Validation: a result provides a contribution to chemical knowledge, but is poor quality
- Validation: to support a 'grand' claim
- To back up modelling of disorder, twinning, incommensurate, modulated structures
- To back up modelling of diffuse scattering
- To make available e.g. disorder, twinning, incommensurate, modulated, diffuse scattering datasets so others can attempt to resolve them
- To support 'Advanced Experiments' e.g. charge density, high pressure, phase transition, gas environment, excited states
- When it is clear that future improvement may be possible through developments in software and modelling
- Training sets/benchmarking for software/methods developers

The survey will take just a few minutes to complete the following multichoice/option format questions:

- If you don't archive raw data, what are the main reasons?
- Where do you keep your raw data?
- Do you manage your archive?
- Is your raw data searchable?
- Is your raw data externally available?
- If it were to become policy to make funded-research raw diffraction data accessible after three years since measurement, would you endeavour to comply?
- Are there any organisations that might have a controlling hand in your research that have a policy mandating you to manage and/or share your raw data?
- Would you anticipate being able to pay for external archive/repository services and facilities e.g. through research grants or institutional funding?
- How likely is it that you will need to revisit raw data in your own work?
- How likely is it that you will need to examine raw data when reviewing someone else's work?
- If you had access to a repository containing raw data, what would you want to use it for?
- In what situations do you feel publishing raw data may be necessary?
- The description that best fits my role is ...
- I come from ...

The survey can be accessed [here](#) and will close on 1 March 2019.

We would like to thank you in advance for helping us understand this complex topic and we aim to communicate the results by mid-2019.

Simon Coles (National Crystallography Service, University of Southampton, UK)

Amy Sarjeant (Cambridge Crystallographic Data Centre, USA)

IUCR ACTIVITIES

The IUCr/OUP Book Series: overview and update

John R. Helliwell



I am glad of the opportunity to highlight details of the [IUCr/Oxford University Press \(OUP\) Book Series](#) in the *IUCr Newsletter*. I presented a poster at the BCA Spring Meeting in Warwick, UK, in April 2018, and a talk in the Education Microsymposium at ECM31 in Oviedo, Spain, in August 2018. The slides for my talk can be found at the IUCr website [here](#).

First and foremost let me say that the IUCr/OUP Book Series Committee warmly welcomes proposals for new publications and makes its recommendations to the IUCr Executive Committee and to the Delegates of the OUP (the body responsible for approving all publications handled by the OUP).

The 60 books published within the Series stretch back about 20 years, and around 60,000 copies have been sold. They are now commissioned in two categories:

- Monographs on Crystallography
- Texts on Crystallography

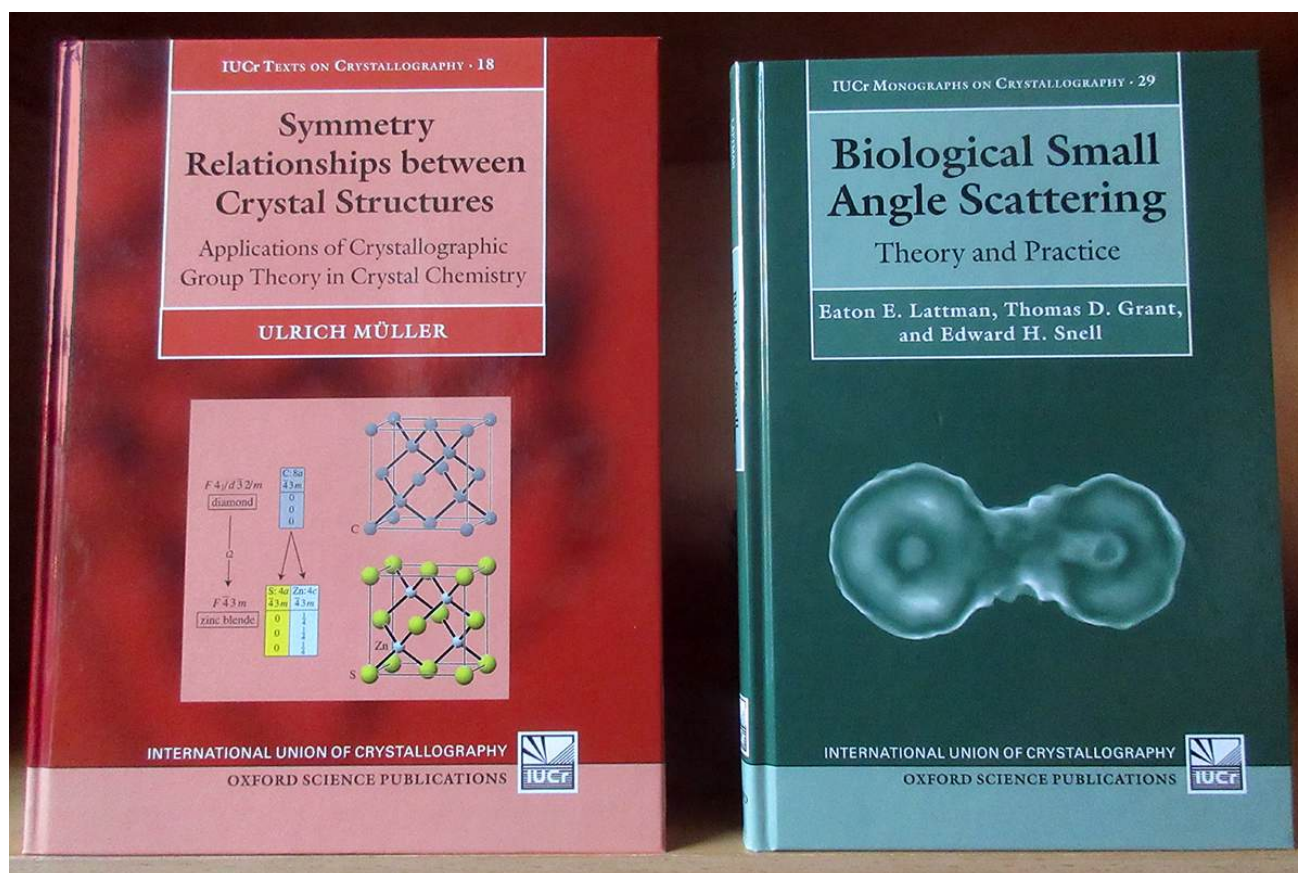
A diverse, highly experienced membership of the Committee has recently been assembled:

- J.R. Helliwell (Chair, UK)
- G. Chapuis (Switzerland)
- J. Gulbis (Australia)
- R. Herbst-Irmer (Germany)

- H. Maynard-Casely (Australia)
- P. Mueller (USA)
- M. Nespolo (France)
- N. Yagi (Japan)
- X. Zou (Sweden)
- K.A. Kantardjieff (USA; *ex officio* as Chair of the IUCr Commission on Crystallographic Teaching)
- S. Adlung and H. Konishi (*ex officio* representatives of OUP)

The procedure to submit a proposal is described [here](#) and basically involves providing:

- a presentation of the motivation, aims, scope, level and readership of the proposed volume;
- a detailed Table of Contents (with subheadings);
- a short CV of the author(s);
- a sample chapter or part of a chapter;
- a list of related books and brief comments on how they differ from that proposed.



The book covers show a consistent and distinctive style, with that on the right showing the latest addition to the Series.

My talk in Oviedo generated an interesting point of discussion regarding our crystallography teaching texts: if a class of students wishes to access simultaneously, e.g. via their University Library, the electronic version of the book, or specific chapters, was that possible? Of course a class might mean, say, 30 students or 200. Does each student need to buy the book (in their preferred format, print or electronic)? I said I would find out Our IUCr/OUP Book Series Committee Member Harriet Konishi looked into it. She stated “*The answer to your question is not very straightforward. Libraries don’t purchase ebooks in the way that you would on Amazon. Instead, at least with OUP, they purchase a subscription to an online offering of our books, which is called [Oxford Scholarship Online \(OSO\)](#). This subscription varies depending on the library, e.g. which kind of or set of books they wish to subscribe to. The library can also choose the level of concurrency (so how many users can access the site at once) at the point they decide to subscribe to or purchase content. One of those options is an unlimited number, which most large universities tend to go for (for obvious reasons), so any number of students can access*

the content at once. But it's up to the individual library to decide that. Individual chapters or the entire book may be viewed through your library's catalogue if they have a subscription."

XXIV IUCr Congress: Microsymposium reports



Instrumentation techniques and/or Computation

MS-006: Computational materials design

Chairs: Samrath Lal Chaplot and Artem R. Oganov

The microsymposium had six excellent presentations that spanned a broad range of computational studies and addressed important issues such as the topological structures, dynamics, algorithms, machine learning, predictions and classification of important features. Eugeny Alexandrov talked about multilevel topological analysis and creation of a knowledge database that could be useful in the design of coordination networks. Matthew Dunstan explained methods of effective screening of databases of crystal structures to design materials especially for carbon capture and storage, and oxygen ionic conductivity. Sandro Scandolo talked about high-pressure studies of SiO_2 , highlighting the atomistic pathways in transitions to metastable crystalline and amorphous structures. Jonathan Skelton made a lucid presentation on the role of lattice dynamics in materials modelling and design. Ivan Kruglov explained machine-learning algorithms to derive interatomic potentials and used it in the evolutionary algorithm *USPEX* to investigate the phase diagram of uranium. John Rodgers talked about extensive use of databases and computation including machine-learning methods in materials design and discovery. Overall, it was indeed interesting to listen through various talks that brought out how the microscopic understanding of structure and dynamics is now applied to predictions of new materials with desired properties that could be tested by experiment.

MS-013: Quantitative electron imaging and tomography

Chairs: Andreas Rosenauer and Eric Van Cappellen

This microsymposium focused on exciting new developments in the field of quantitative transmission electron microscopy. The first two invited talks presented by Ivan Lazic and Knut Müller-Caspary demonstrated measurement of the momentum transfer from which the electrostatic specimen potential, atomic electric field and charge density can be obtained with sub-ångström spatial resolution. The first technique uses a segmented detector, the second a pixelated detector. A third approach to measure the phase of the object function and thus the specimen potential was shown by Peter Nellist, who demonstrated detection of charge transfer from the B to the N site in hBN. The third invited talk presented by Georg Haberfehlner shed light on the state of the art in electron tomography, demonstrating 3D reconstruction of atomic structure and of composition with spectroscopic techniques.

First experiments towards 3D measurement of strain with electron tomography were shown in the talk by Duncan N. Johnstone.

MS-024: NMR crystallography and related methods

Chair: Manish Mehta

This microsymposium, featuring six leading practitioners in the emerging field of NMR crystallography, was held on the Wednesday morning of the Congress. It came on the heels of a successful keynote lecture by David Bryce on the Tuesday evening titled, “Structure and Properties of Materials by Solid-State Nuclear Magnetic Resonance Observables.” (That keynote had over 60 members in the audience.) Both the keynote and the microsymposium were the first of their kind at an IUCr Congress. At its peak, the microsymposium had nearly 60 members in the audience. NMR crystallography, while an emerging discipline, is broad in its scope, ranging from technique development to applications in a variety of areas. The six presentations reflected this breadth in an impressive way, and those who stayed for the full session came away with an appreciation of the scope of the field as well as its direction. The talks were not too technical - which they could easily have been - and were broadly accessible to the audience. On a procedural matter, all speakers kept their talks within the advertised time limits, and they stuck to the advertised talk titles. The presentations were of a complementary nature and gave a good feel for the questions that are being addressed and the tools employed to tackle those questions. P.K. Madhu gave an excellent overview of cutting-edge NMR capabilities and their potential application to crystallography, while Yusuke Nishiyama showed what can be accomplished with proton chemical shift tensors. Sachin Chaudhari, who has just completed a postdoc with Lyndon Emsley in Lyon, spoke about the utility of dynamic nuclear polarization, while James Harper spoke about the possibility of determining crystal structures using NMR data alone. Gerd Buntkowsky and Jurgen Senker spoke about powerful applications of NMR crystallography in the study of enzymes and polymer additives, respectively. In all, this was a highly successful microsymposium, which made a valuable addition to the overall scientific programme.

MS-050: Small angle scattering studies of biomacromolecular kinetics

Chairs: Pau Bernado and Clement Blanchet

This microsymposium assembled presentations that reflect the present progress of SAXS, which has become an essential tool to structurally characterize biomolecules in solution. The novel experimental setups presented allow the monitoring of complex biological phenomena or the recording of new observables to structurally probe biomolecules. Two speakers presented the current developments on their beamlines. Automated sample collection and chromatography coupled with SAXS available on the BM29 beamline (ESRF, Grenoble) were presented, together with the plans for the future upgrade at the ESRF. The presentation of the P12 beamline (EMBL/PETRAIII, Hamburg) focused on the opportunities in anomalous SAXS and time-resolved experiments. The high-flux option at the P12 beamline, allowing the collection of data at the sub-ms time scale, is particularly interesting for time-resolved studies of biomacromolecular kinetics. Two presentations focused on the application of SAXS for the study of complex biological phenomena covering multi-component equilibria in biological systems and in crystallisation processes. Interestingly, both studies were made possible through the development of microfluidic sample environments, which have a growing impact on modern synchrotron SAXS beamlines. The new data collected on these setups will foster the development of theoretical approaches for their interpretation from a structural perspective.

MS-059: Quantitative electron diffraction

Chairs: Mauro Gemmi and Enrico Mugnaioli



Speakers and chairs (l-r): Artem Abakumov, Lukas Palatinus, Mauro Gemmi, Enrico Mugnaioli, Stef Smeets, Katariina Pussi and Koji Yonekura.

This microsymposium has confirmed the growing interest in electron crystallography, attested by the remarkable number of participants. The broad range of methods and applications presented by lecturers displayed that this field is in continuous and fast expansion. Results from the first *in situ* electron diffraction tomography (EDT) experiment on a Li-containing nanodevice during a charge cycle were shown, which allowed an estimation of the variation of the Li occupancy at different crystallographic sites. The recently developed dynamical refinement method has been extended to modulated crystal structures with the introduction of new criteria for reflection assignment and sorting. Electron diffraction tomography may now also be applied to protein nanocrystals. Novel results show that energy-filtered EDT data allowed not only the solution of the protein structure with atomic resolution, but also the detection of its charged states. The expansion of electron crystallography into all the classical fields of crystallography is endorsing electron crystallography as the eligible technique for any structural problem at the nanoscale.

MS-068: New X-ray sources: storage rings, FELs and laser-based

Chairs: Tetsuya Ishikawa and Harald Reichert

Over the past two decades, we have seen great strides in the advancement of X-ray source technology with about 50 facilities operational worldwide today. Now we are facing the transition of storage-ring technology from double-bend-achromat (DBA) to multi-bend-achromat (MBA) lattices for smaller horizontal electron-beam emittance. At the same time, X-ray free-electron lasing (XFEL) has been

achieved using self-amplified spontaneous emission (SASE) technology. In 2005, the FEL, FLASH at DESY, Germany, started operation in the soft X-ray range, followed in 2009 by the first XFEL in the hard X-ray range at the LCLS in Stanford, California, USA, and in 2011 by SACLA at Harima, Japan. This year brought three new XFEL facilities on the stage in Germany, Switzerland and South Korea. In addition, several new types of laser-based X-ray sources are currently under development. The microsymposium was organized by Harald Reichert (ESRF) and Tetsuya Ishikawa (SPring-8/SACLA). It featured three invited speakers providing a review of developments in synchrotron radiation sources, XFEL sources and laser-based sources. In addition, four contributing speakers addressed the following topics: (i) the first MBA machine, MAX-IV, at Lund; (ii) the newly emerging European XFEL; (iii) recent progress in lab-based sources; and (iv) the Kurchatov synchrotron radiation source, which until recently was not widely known. Joel D. Brock of Cornell U., who serves as the director of Cornell High Energy Synchrotron Source (CHESS), gave an overview of existing storage-ring sources as well as planned upgrades and future facilities. He discussed the general scientific implications of the transition to MBA-based technology. Robert Feidenhans'l, the Chairman of the Management Board of the European XFEL GmbH, changed his topic from an overview of SASE-based XFELs to a status update on the European XFEL, because it recently succeeded in lasing and is nearly ready to start user operations. Tetsuya Kawachi of the National Institute for Quantum and Radiological Science and Technology in Japan discussed laser-based X-ray sources through both higher harmonic generation (HHG) and plasma emission. For the first contributing presentation, Marjolein Thunnissen reported on structural biology at MAX-IV, the world's first operational MBA-based storage ring. She not only discussed structural biology, but also shared the latest results from her facility. Next, Alexander Blagov presented an overview of future imaging and diffraction research at the European XFEL. Although some parts of his presentation overlapped with Professor Feidenhans'l's talk, Dr Blagov provided interesting details on the introduction of Russian contributions to the European XFEL. Vernon Smith of the Bruker Corporation gave the third contributing presentation on the topic of laboratory X-ray sources. He reviewed several recent developments achieved by the Bruker Corporation, including a macromolecular crystal structure analysis system. The last talk was given by Roman Senin of the Kurchatov Institute in Russia. He provided an introduction to the Kurchatov synchrotron radiation facility, which has generally not been accessible to scientists outside of Russia. Despite the concurrent topics on crystallography, many audiences participated in this microsymposium. In fact, some of the talks drew standing-room-only participants. In the future, additional consideration should be paid to the size of the meeting rooms and the number of chairs available.

MS-076: Diffuse scattering in crystalline structures

Chairs: Ray Withers and Bernardo Barbiellini

This session was very well attended throughout. It opened with a highly entertaining and informative talk from Andrew Goodwin using tiling to show how even strict local rules need not lead to long-range periodicity. The widespread class of highly correlated disordered materials (including ices, spin glasses, ferroelectrics) and their consequences for physical properties were highlighted and well illustrated. Marek Pasciak then beautifully illustrated the use of large multi-scale molecular dynamics simulations of detailed experimental diffuse scattering data to reliably extract time and space resolved polar fluctuations from four separate ferroic and piezoelectric materials systems. The obtained fits to the observed diffuse scattering data were most impressive. Thomas Weber presented a detailed analysis of the diffuse scattering data characteristic of PbTe, a leading thermoelectric material. This analysis was based on state-of-the art software developed at ETH Zurich for robustly simulating 3D pair correlation distributions. Arkady Simonov illustrated some exciting examples of diffuse scattering spectra where the phase problem could be solved. He also pointed out the existence of a planar extinction condition in reciprocal space and even determined a space-group symmetry for an experimental diffuse distribution. This work opens new opportunities to phase and thereby extract faithful reconstructions in real space from diffuse scattering data. Patrick Tung presented detailed diffuse scattering data of piezoelectric NBT-

BT materials under applied electric fields from experiments performed at the ESRF. Big box Monte Carlo simulations were used in order to analyze the experimental data in term of ordered disorder. Ella Schmidt presented an ingenious fitting method for studying diffuse scattering. The method introduced molecular form factors and thus dramatically reduced the computational effort required with respect to standard brute force Monte Carlo simulations.

MS-077: Coherence, spectroscopy and time resolved crystallography with new sources

Chair: Jan Kern

The microsymposium covered a large range of techniques as well as samples studied, illustrating the wide application of time-resolved X-ray techniques using new experimental approaches. These ranged from X-ray spectroscopy with tens of fs time resolution at SACLA (Katayama, SACLA) through elucidation of details of protein-cofactor interactions in time-resolved fs crystallography (Standfuss, Paul-Scherrer Institute), the progression of electric potential induced density waves in alloys studied in the hundreds of fs time range using slicing techniques at synchrotron sources (Ravy, University of Paris) to slower time-resolved diffraction experiments in the microsecond timescale conducted on organic molecules at home sources (Basuroy, SUNY Buffalo). A common theme in most of the talks was the important role of new enabling technology to perform these demanding experiments, for example advanced beam analytics at SACLA to reduce the timing jitter in ultrafast time-resolved experiments (Katayama), the transfer of sample-delivery methods developed for XFEL experiments into synchrotron experiments (Standfuss) or the development of novel ultrafast read-out detectors like the EIGER (presented by Brandstetter, Dectris Ltd). The audience covered a wide range of expertise (materials science, physics, X-ray spectroscopy, structural biology), making for a lively discussion following each of the presentations.

MS-103: Methods for characterizing commensurate and incommensurate magnetic structures

Chairs: F. Damay and M. Henriques

Despite the difficulties encountered during its organisation (mainly because of the lack of submitted abstracts), this microsymposium, although not quite dedicated to technical methods as advertised in its title, was a very stimulating and successful one. The five speakers gave very good quality talks, and gave very interesting examples of alternative techniques [such as Mössbauer spectroscopy, to identify $S=0$ spins (Ling)] to solve magnetic structures when neutron scattering gives equally likely possible solutions. A variety of different materials, ranging from magnetoelectrics to thermoelectrics, were presented, broadening the interest of the audience. The invited speaker, Stephen Collins from Diamond (UK), gave a particularly interesting talk on the specifics of resonant and non-resonant X-ray scattering techniques, applied to investigate the subtleties of magnetic structures (like very small spin canting), which cannot be fully apprehended by neutron diffraction. His presentation on the possibility of using Compton scattering - an inelastic X-ray scattering process that yields a projection of the electron momentum density - to probe magnetoelectrical properties, could have a lot of impact on this field in the nearby future to identify unambiguously time reversal or space inversion in crystal structures. Overall the session was well attended, and a good synergy between the attendees and the speakers was noticed.

MS-112: Laboratory sources vs. large scale facilities for charge density studies

Chairs: Regine Herbst-Irmer and Jacob Overgaard

In this microsymposium six speakers presented experimental charge-density investigations into inorganic materials, organic small molecules and proteins using powder or single-crystal data collected either in the lab or at synchrotrons. Mads Jørgensen (Aarhus University, Denmark) described the investigation on powder with the new 'Aarhus Vacuum Imaging Plate Diffractometer'. Then Nicolas Claiser (Université de Lorraine, France) compared two single-crystal data sets of YTiO_3 collected at Bruker (Karlsruhe) and at SPring-8. Parthapratiim Munshi (Shiv Nadar University, Tehsil Dadri, India) presented a review of charge-density studies in small molecules and proteins and reported on the new developments in detector technology. Krzysztof Wozniak (University of Warsaw, Poland) talked about precision and accuracy of single-crystal X-ray results, comparing the Independent Atom Model, the Multipole Model, Hirshfeld Atom Refinement and the Transferable Aspherical Atom Model of electron density. Eiji Nishibori (University of Tsukuba, Japan) described the charge-density investigations of LaB_6 and BaB_6 using powder data collected at SPring-8. Finally, Hidetaka Kasai (University of Tsukuba, Japan) spoke about a charge-density study of TiS_2 using single-crystal data collected at SPring-8.

Materials and minerals

MS-070: Superconducting materials

Chairs: Irina Makarova and Rob McQueeney

The discovery of a new class of high-temperature Fe-based superconductors has attracted substantial attention in the scientific community due to providing a new platform for investigations of superconductivity as a phenomenon. MS-070 was dedicated to the crystallography of these superconducting materials, their properties and different aspects of formation. E. V. Antipov (Russia) demonstrated the possibility of the increase of the superconducting transition temperature in $\text{Fe}_{1+\delta}\text{Se}$ by more than 30 K by the modification of the crystal structure. Such modification could be performed by the intercalation of Li, Fe or alkaline cations like K in the interlayer space. The data obtained in that study revealed a remarkable new opportunity for Tc-enhancement. A. L. Vasiliev (Russia) introduced the study of low-temperature Nb_3Sn based superconductors used for the manufacture of magnetic coils for ITER and LHC projects by means of electron microscopy, including transmission/scanning electron microscopy, nano-electron diffraction and microanalysis, and new data on the microstructure of Gd-Ba-Cu-O layers doped with Sn and Zr in order to obtain pinning centers and on the structure of iron chalcogenide single crystals and thin films including three-dimensional reconstructions. S. Nandi (India) reported data on Eu-based Fe pnictides obtained by X-ray resonant magnetic scattering, and polarized and unpolarized neutron diffraction. The advantages of these experimental techniques for smart materials research were also noticeably shown. The highly sensitive EXAFS for obtaining precise structural data was discussed by S. M. Heald (USA).

MS-097: Functional magnetic materials

Chairs: D. Shoemaker and J. A. Alonso

In this microsymposium, the speakers covered different, complementary aspects of the topic "functional magnetic materials". J. Cumby (UK) presented an ellipsoidal method for quantifying octahedral distortions in ionic compounds and applied this analysis to magnetite below its Verwey transition. The distribution of ellipses affords a view of the correlations between distortions of neighboring octahedra in

“trimerons” in the structure. Applying this method to data-mined sets of Fe^{3+} -O compounds revealed a tendency for the cation to off-center, likely due to second-order Jahn-Teller effects from their $3d^5$ electron configurations. J. Garcia-Muñoz (Spain) and H. Kobayashi (Japan) presented complex magnetoelectric interactions in cobaltates and EuNiO_3 , respectively. B. Kennedy (Australia) discussed the interplay of ionic size and spin-orbit coupling in ordered double perovskites containing Ru, Ir and Os. S. Peter (India) introduced novel structures of rare-earth-containing intermetallics and their magnetic properties and transport.

Physical and/or fundamental

MS-017: Extending the boundaries of crystallography

Chairs: Manuel Loquias and Mois I. Aroyo

The microsymposium dealt with recent novel advances in both theoretical and experimental aspects of crystallography. Walter Steurer of ETH Zurich opened the session by giving a talk on the state of the art of research in the structure, formation and growth of quasicrystals and, in particular, of intermetallic quasicrystals. In addition, he gave his perspectives on the immediate goals and challenges in quasicrystal research. The next talk, by Stephen Timothy Hyde of the Australian National University, was on the taxonomy of hyperbolic orbifolds and its application to triply periodic minimal surfaces. The last invited talk, by Tomonari Dotera of Kindai University, Japan, supplemented the previous talks: he discussed self-similar tilings and quasicrystals associated to the bronze mean, and their results on crystal structures on triply periodic minimal surfaces obtained *via* Monte Carlo simulations of hard spheres. There were three contributed talks to the microsymposium. Alistair Overy presented models to study the relationship between disordered entanglements and swelling in fibrous materials. The talk by Espen Drath Bojesen described how scanning electron nanodiffraction (END) may be used to distinguish between seemingly similar amorphous materials. Finally, Lorraine Andrade Malaspina reported on efforts to map the trajectory of proton transfer in different hydrogen maleate salts with varying symmetry of hydrogen bonds.

MS-035: Crystal structure relations and applications

Chairs: Wolfgang Schmahl and Valeriy Talanov



Speakers and chairs (l-r): Valeriy Talanov (Russia, co-chair), Stefan Adams (Singapore), Branton Campbell (USA), Dhananjai Pandey (India), Gervais Chapuis (Switzerland), Sergey Krivovichev (Russia), Swastik Mondal (India) and Wolfgang Schmahl (Germany, co-chair).

This microsymposium induced great interest among the participants of the Congress. Among the speakers were outstanding scientists Gervais Chapuis (Switzerland), Sergey V. Krivovichev (Russia), Branton Campbell (USA), Dhananjai Pandey (India), Stefan Adams (Singapore) and Swastik Mondal (India). In his presentation, Gervais Chapuis considered the superspace concept in applications to crystal chemistry of structural families and polytypes. Sergey V. Krivovichev outlined the original concept of information-based measures of structural complexity of crystals, and discussed the evolution of various natural and synthetic phase systems in this respect. Branton Campbell presented an algebraic approach to identification of rotational rigid-unit modes wherein the conditions of connectedness are used to construct a linear system of equations in the rotational symmetry mode amplitudes. Dhananjai Pandey presented unambiguous evidence for an iso-symmetric phase transition involving coupled order parameters in CaTiO_3 . Stefan Adams discussed his approach to determine bond-softness adapted bond-valence parameters based on a description of bond valence as a function of valence electron density. Swastik Mondal spoke about a new insight into the bonding mechanism of boron carbide that helps to explain why boron carbide and related materials can preserve the same crystal structure over a range of compositions.

MS-098: Recent advances in quasicrystal research

Chairs: Katariina Pussi and Yasushi Ishii

In the session six talks were given, out of which two were invited and four contributed. The session gave a nice overview of the field including talks on both theoretical aspects and experimental studies. In the first invited talk, theoretical tiling models and a new inflation rule for generating canonical cell tilings were discussed by Nobuhida Fudita (Sendai, Japan). The second invited talk, given by Julia Dshemuchadse (University of Michigan, USA), also presented theoretical aspects, including crystal

structures in soft matter and new structure types built by packing polyhedra. One of the contributed talks explicitly brought up the universal question of “from structure to the physical properties – how far can we go?”. This nicely summarizes one of the main targets of quasicrystal research, which was visible in all of the talks in this microsymposium. Subjects covered in other contributed talks included quasiperiodically arranged molecular thin films, icosahedral quasicrystals with rare earth atoms and γ -brass related complex phases in Rh-Cd binary systems.

MS-125: Small-angle scattering data formats, standards and repositories

Chairs: Cy Jeffries and Manfred Roessle

The microsymposium encompassed a number of topics relevant to the standardization practices in the field of small-angle scattering (SAS), with a particular emphasis on biological solution scattering. Alexey Kikhney (EMBL) presented the Small-Angle Scattering Biological Data Bank (SASBDB; sasbdb.org), the largest publicly accessible repository of bioSAS data and models, which included recent SASBDB-PDB developments (integration of SAS into the PDB OneDep system) and new visualisation tools for data quality assessment (‘sliders’). The sliders drew lively discussions from the audience. Brinda Vallat (Rutgers/PDB) detailed the complexities of capturing experimental results and metadata derived from hybrid methods using the CIF file format (dictionaries/ontology). An alternative, fully adaptable system, NXcanSAS (cansas.org), was presented by Pete Jemian (ANL). Combined, these talks highlighted the immense challenges facing the curators of databases where both SAS and hybrid methods are deposited in parallel. Andrew Allen (NIST) gave a rigorous (and important) talk on the development of an internationally recognised glassy-carbon standard for the absolute scaling of scattering intensities. The MS was concluded by Mitchell Guss (USyd) who outlined recommendations for publishing bioSAS data and models described by Trehwella *et al.* that were published during the IUCr2017 Congress [*Acta Cryst. D73*, 710-728 (2017)].

Special activities

MS-021: Terminology issues in crystal engineering

Chairs: Carol Brock and Christer Aakeröy

Prior to IUCr2017, the chairs of this session were more than a little apprehensive; would anyone show up for a 2.5-hour symposium dedicated exclusively to terminology issues in crystal engineering? The answer was a resounding ‘Yes!’, as the 250-seat lecture hall was nearly filled for each of the five talks. The session also managed to live up to the billing (as stated in the *IUCr Newsletter*) of providing a “...popular, lively and indeed humorous session”. Desiraju and Metrangolo delivered detailed insight into how the IUPAC definitions of the hydrogen bond and the halogen bond, respectively, have been arrived at. The time and effort that go into developing appropriate nomenclature that is acceptable by the community are clearly considerable. MacGillivray examined some practical and legal pitfalls that can arise as a result of polymorphism, and terminology resides at the core of many of those issues. Vittal gave an entertaining overview of the frequently entangled descriptions that surround coordination polymers and/or metal-organic frameworks (covering acronyms from MOFs to ZIFs *via* PIZOFs). Finally, Aakeröy illustrated, with a series of often amusing examples, some of the challenges in deciding exactly what types of solids should be called co-crystals.

MS-032: Crystallography courses around the world

Chairs: Annalisa Guerri and Juan Manuel García-Ruiz

Within a room overcrowded with a participative audience, MS-032 hosted 16 excellent presentations (half of them as posters) on the efforts of our community in teaching crystallography. Several lectures reported the initiatives of the IUCr Regional Associates, including LACA (Diego Lamas), ACA (Amy Sarjeant) and ECA (Alessia Bacchi), along with a report about crystallographic courses in Africa by Andreas Roodt. We heard several presentations on specific Schools, such as the European Master of Crystallography, a one-year master involving different countries in Europe (Fermín Otálora); the FEBS crystallization courses running since 2004 in the Czech Republic (Ivana Smatanova); and the International Schools of Crystallization of Granada, Spain, since 2006 (Jaime Gomez-Morales). Michele Zema reported about the OpenLab courses from North Africa to the Far East and South America, a project born in 2014 for the IYCr and still expanding. Dubravka Jung covered the connection between teaching and industry. Courses on materials physics (Peter Moeck), symmetry (Massimo Nespolo), macromolecular structures (Ruslan Sanishvili) and for undergraduate students (Cora Lind-Kovacs) were also reported. The programme was completed with discussions about the IUCr crystal growing competition (Luc Van Meervelt), the Instituto Rocasolano website (Juan A. Hermoso) and educational initiatives in Croatia (Aleksandar Visnjevac).

MS-044: Structural databases as teaching tools - Part A (macromolecules)

Chairs: Joel Sussman and Christine Zardecki

Free public access to structural data and related bioinformatics resources enables a wide variety of educational resources as presented in MS-044. Jaime Prilusky (Israel) demonstrated how simple Proteopedia webpages enlighten macromolecular structure-function relationships for students and researchers. More than 130,000 PDB entries, as well as thousands of user-added pages, can be explored by clicking on text to highlight the corresponding feature in 3D, e.g. a tutorial “How do we get the oxygen we breathe” designed for high school and beginning college students. Shuchismita Dutta (USA) described how looking at disease through a structural biology perspective promotes development of RCSB PDB resources aimed at high school and undergraduate students. In bioinformatics studies, Masters students have used PDB virus structures for analysis and compiled them into specialized prediction databases, leading to an *in silico* pipeline for vaccine development under the direction of Urmila Kulkarni-Kale (India). At Protein Data Bank in Europe, Sameer Velankar (UK) and his team have used everything from art to topology map depictions as a way of bringing structure to biology and beyond. Alexey Kikhney (Germany) demonstrated how the SASBDB and DARA resources are extremely useful biological solution scattering teaching tools, as well as for getting an initial idea of the overall structure of an unknown protein or protein complex. In the final presentation, Hirofumi Suzuki (Japan) wore red-cyan glasses while demonstrating how playing with 3D biomolecular structures is easy and fun using PC, mobile and VR software tools hosted by Protein Data Bank in Japan.

MS-099: Crystallographic data and structure validation from data collection to publication - IUCr setting standards

Chairs: Anthony Linden and Wladek Minor

Five speakers presented different aspects of data validation and data archiving. We have come a long way from publishing printed copies of structure factor tables within journal articles to the full electronic deposition of diffraction data and even diffraction images, because this not only allows the validation of results, but is a full archive that permits interested persons to extract information not thought about or

even possible at the time of the original work. Ton Spek (The Netherlands) summed up the aim of validation clearly: *results are valid if all data are included and the authors document what was done during the experiment and the thinking behind the decisions made*. Loes Kroon-Batenburg (The Netherlands) indicated that the archiving of frame data needs not only public data depositories to cope with the quantity of data, but also the deposition of full metadata, without which it is difficult to reprocess data. Jim Simpson (New Zealand) recounted the discovery of fraudulent crystal structures and how validation tests were expanded to reveal such manipulations. DFT-D calculations can now be used to check the validity of structures determined from XRPD (Jacco van de Streek, Germany). Common issues are poor refinement but structure correct, H-atom errors and element swap errors, as well as the importance of the consideration of preferred orientation. Finally, John Westbrook (USA) described the wwPDB OneDep Validation procedure during deposition of macromolecular structures.

CRYSTALLOGRAPHY IN AFRICA

The future is crystalline for Benin: An interview with Thierry d'Almeida

Michele ZemaSekazi K. MtingwaSandro Scandolo



We had a chance for an informal chat with Dr Thierry d'Almeida at the end of one of the numerous meetings of the LAAAMP Executive Committee, when Thierry was invited to discuss the strategies and plan future activities for the development of crystallography and synchrotron-related disciplines in Benin and neighbouring countries. Thierry, who is originally from Benin and works at the CEA (Commissariat à l'Energie Atomique et aux Energies Alternatives, France), was introduced to the LAAAMP Executive Committee by Herman Winick. He immediately impressed us with his enthusiasm and dedication to the cause of improving scientific education and research in Africa as a way for achieving socioeconomic progress, and was eventually selected to deliver a series of presentations as part of the Colloquium Programme of [LAAAMP](#) (Lightsources for Africa, the Americas, Asia and Middle-East Project), a joint IUPAP-IUCr project funded under the 2016-2019 ICSU Grants Programme.

Following the successful [LAAAMP Colloquium](#) delivered in Cotonou in the period 2 to 5 May 2018, Thierry was invited to spend two weeks in his home country of Benin meeting with President Patrice Talon, his Cabinet and numerous other dignitaries to discuss both LAAAMP and the newly proposed crystallography lab and training programme called XTech-SD (X-Ray Techniques for Sustainable Development).

Q: Thierry, let's start with XTech-SD? Tell us more about this project.

A: XTech-SD is a project that I designed with Dr Marielle Agbahoungbata, a young chemist from the University of Abomey-Calavi in Benin. The overall objective of the project is to endow the local and regional scientific communities with technical skills that will allow them to use X-ray techniques as tools for solving specific critical socioeconomic issues. The training programme is being implemented in collaboration with [LAAAMP](#) and within the framework of the [IUCr-UNESCO OpenLab](#) and the [IUCr Crystallography in Africa](#) initiatives. We expect to train annually over a hundred Masters and PhD students from Benin and neighbouring countries, such as Nigeria, Togo, Niger and Burkina Faso. We will establish a permanent user research facility with experienced, permanent staff to act as a hub for the region. XTech-SD will have temporary quarters in Cotonou starting from May 2019, but will subsequently relocate to Sèmè City from 2021.

Q: What is Sèmè City?

A: Sèmè City is the International City dedicated to Innovation and Knowledge, presently under development in an area located between Cotonou and Porto-Novo. The project was launched as part of “[Revealing Benin](#)”, a transformative large-scale investment programme launched in December 2016 by President Talon and the Government of Benin. Sèmè City houses and promotes synergies between elite educational establishments, research and development centres, and acts as a business incubator. We hope that XTech-SD will become an important asset of Sèmè City.

**Q: You met with President Talon and his Cabinet. What was their reaction when you mentioned crystallography and advanced light sources?**

A: There were two separate meetings, one with President Talon and another one with the Cabinet. I had one hour on schedule to talk with President Talon and we ended up talking for more than two hours. He was keen to learn everything about all our initiatives. I discovered a man who is perfectly aware of the challenges and who has a clear roadmap in his mind. President Talon stated that he was already aware of the [LAAAMP](#) project and will spread the word among his fellow Presidents. His government is ready to support XTech-SD as well as the next joint Pan African Conference on Crystallography and African Light Source Conference ([PCCr2/AfLS2, Accra, Ghana, 28 January-2 February 2019](#)).

When I met with the Cabinet, I gave a full presentation about [LAAAMP](#) and Advanced Light Sources, which was well received by the Ministries. Dr Marie Odile Attanasso, Benin's Minister of Higher Education

and Scientific Research, remarked that these were just the type of programmes that they have been waiting for.

Q: How important was your *LAAAMP* Colloquium Programme to ‘spread the word’ and foster such initiatives?

A: My first trip to Benin last May was extremely rewarding, far beyond my expectations. Most people I met, and these were scientists, had only a vague idea about Advanced Light Sources, and were almost totally unaware of the *LAAAMP* initiative. I met people of different backgrounds (chemistry, biochemistry, physics, mathematics and geology) from the two major universities of the country, Abomey-Calavi in Cotonou and IMSP (*Institut de Mathématiques et Sciences Physiques*) in Porto-Novo, and the Commissioner of Education.

However, my biggest satisfaction came from the young students. I have been impressed and deeply moved by their thirst of knowledge, their determination to grab the opportunity of the prospect of an African Light Source (AfLS) as a way to play an active role in science.

During that first trip, I decided to set up a local, informal AfLS Working Group composed of some of the brightest young faculties (both chemists and physicists), whose main task was to disseminate further synchrotron science among the students and identify specific studies of interest for the local and West African scientific communities that could be submitted as proposals to *LAAAMP*’s Partnering Advanced Light Sources in the near future. Within three months, this initial idea matured and transformed into the XTech-SD initiative.

Q: Did you do all this on your own or are there any persons you want to mention or thank?

A: Many, many people should be mentioned. Of course, the Executive Committee of *LAAAMP* (S. Mtingwa, M. Zema and S. Scandolo) has been and is being very supportive and helpful. Without your initiatives and the idea of having a Colloquium presentation in Benin, none of this would have happened. Jean-Pierre Ezin (founder of the IMSP, Porto-Novo) has been a great facilitator, together with many other locals, among which I want to mention Dr Marielle Agbahoungbata, XTech-SD Project co-Leader, who is presently at University of Zurich with Professor A. Linden and has participated in the IUCr 2017 Congress in Hyderabad, our Working Group at the University of Abomey-Calavi headed by Professor Etienne Sagbo, and all the staff from IMSP.

There is one person who deserves a special mention for making all this happen. This is Claude Borna, the Managing Director of the Sèmè City Development Agency, and Advisor to President Talon. Without her hard work and dedication, we would not have been able to make such significant progress within such a short time period. She was convinced by the unique potential of XTech-SD as a tool for sustainable development and she managed to secure the support of the Government of Benin at the highest level.

Also, I was very lucky to meet Cédric Villani, who is a famous French mathematician and Member of Parliament, who happened to be visiting IMSP during my first trip. We had extensive discussions about the *LAAAMP* and the AfLS initiatives. Cédric met with President Talon the next day and introduced the AfLS. I was immediately contacted by his advisers, who invited me to give an overview of the project, which I did minutes before leaving the country. They eventually reported to the President and this is how the story started.

Q: How did you end up dealing with such projects? Tell us more about yourself and your previous experiences.

A: My initial background as a graduate student was essentially in materials science and solid-state physics with a strong emphasis on crystallography. But it was not until I joined the Institute for Shock Physics at Washington State University more than 20 years ago, after my PhD, that I realized the extraordinary power of X-rays for interrogating matter under various conditions. During that seminal experience, I performed one of the pioneering X-ray diffraction measurements from a solid undergoing a shock-induced structural phase transition. From that time, I never really stopped using X-rays whether during the eight years that I spent at the European Synchrotron in Grenoble as a beamline scientist or later at the Cavendish Lab in Cambridge, or even now at the CEA. I have been convinced for a long time that X-ray techniques can make a real difference in addressing some of the most critical socioeconomic challenges in developing countries and especially in Africa. Being given the opportunity to serve the *LAAAMP* is such an extraordinary fortuitous alignment of stars that I intend to build on in order to get something significant done in Africa.

Q: What are the next steps?

A: We are working hard with the Sèmè City team to have the XTech-SD lab established as soon as possible. We are currently discussing with manufacturing companies to secure all necessary equipment on time. Hopefully, we will be able to have the first two-week training session in May/June 2019 under the framework of the IUCr-UNESCO *LAAAMP* OpenLab initiative. We are planning to have two of these sessions per year directed to 50 students from IMSP plus 60 from other institutions in Benin and neighbouring countries. The course will be part of their curricula. Following a natural trend started by Rwanda in 2008, the teaching will be in English, in order to grow a scientific community prepared to take part in international activities. The XTech-SD Lab will serve as a model of a Feeder Facility for the future African Light Source.

We finally thanked Thierry for his time and encouraging report and wished him every success. He actually transferred a lot of energy and enthusiasm to us. This project is an important step towards the establishment of proper scientific infrastructure in Africa, and also the potential implementation of an African Light Source. It will definitely serve as a model for other African countries.

Thierry's meetings have received extensive press coverage, including television news, which can be found via these links:

https://youtu.be/yUY_54LE8dI

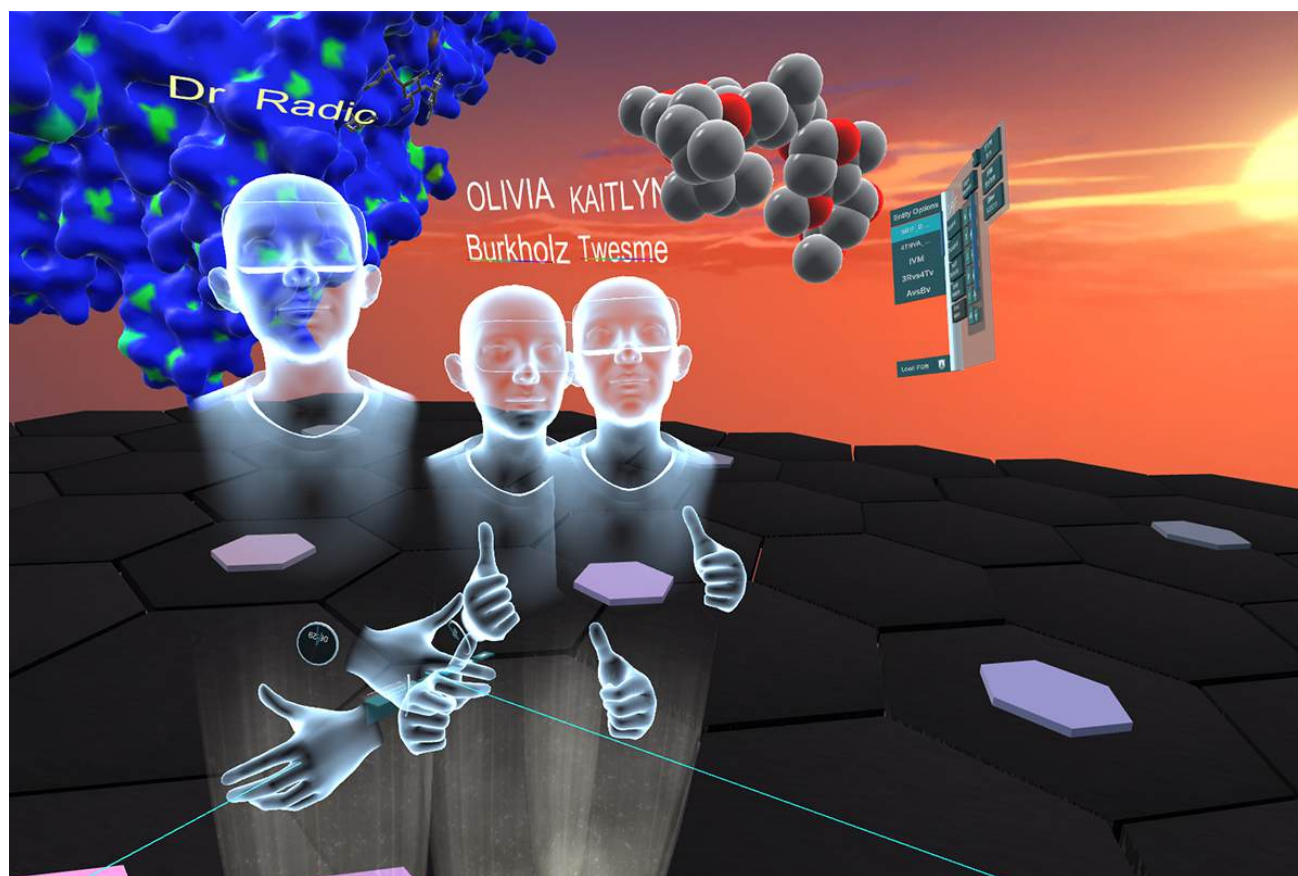
<https://www.flickr.com/photos/presidencebenin/albums/72157698045451852>

<http://boulevard-des-infos.com/2018/09/enseignement-superieuraudience-au-cabinet-de-attanasso-le-professeur-thierry-dalmeida-expose-le-projet-laaamp-au-mesrs>

OUTREACH

Wisconsin Space Crystal Mission

Ilia Guzei



A virtual selfie of protein explorers Dr Zoran Radić and Wisconsin Space Crystal Mission team members Olivia Burkholz (age 18) and Kaitlyn Twesme (age 14).

Are you a high- or middle-school student in Wisconsin, USA? Are you interested in science or arts? If you answered yes or yes, then nothing should stop you from competing for a chance to grow crystals at the International Space Station!

A state-wide Wisconsin Crystal Growing Contest (WICGC) among youths aged 11-18 has been an annual event since 2014 (Figure 1a). Over 650 students and teachers annually compete for prizes awarded based on crystal quality and the students also vie for prizes in the 'crystal-inspired art' category. The event is organized at no cost to participants and is completely supported by sponsors; the IUCr has co-sponsored the project twice since inception. The WICGC (<http://wicgc.chem.wisc.edu/>) has been previously described in the Spring 2015 and Fall 2016 issues of the ACA's newsletter *Reflexions* and herein I will instead briefly describe the WI Space Crystal Mission (Figure 1b).

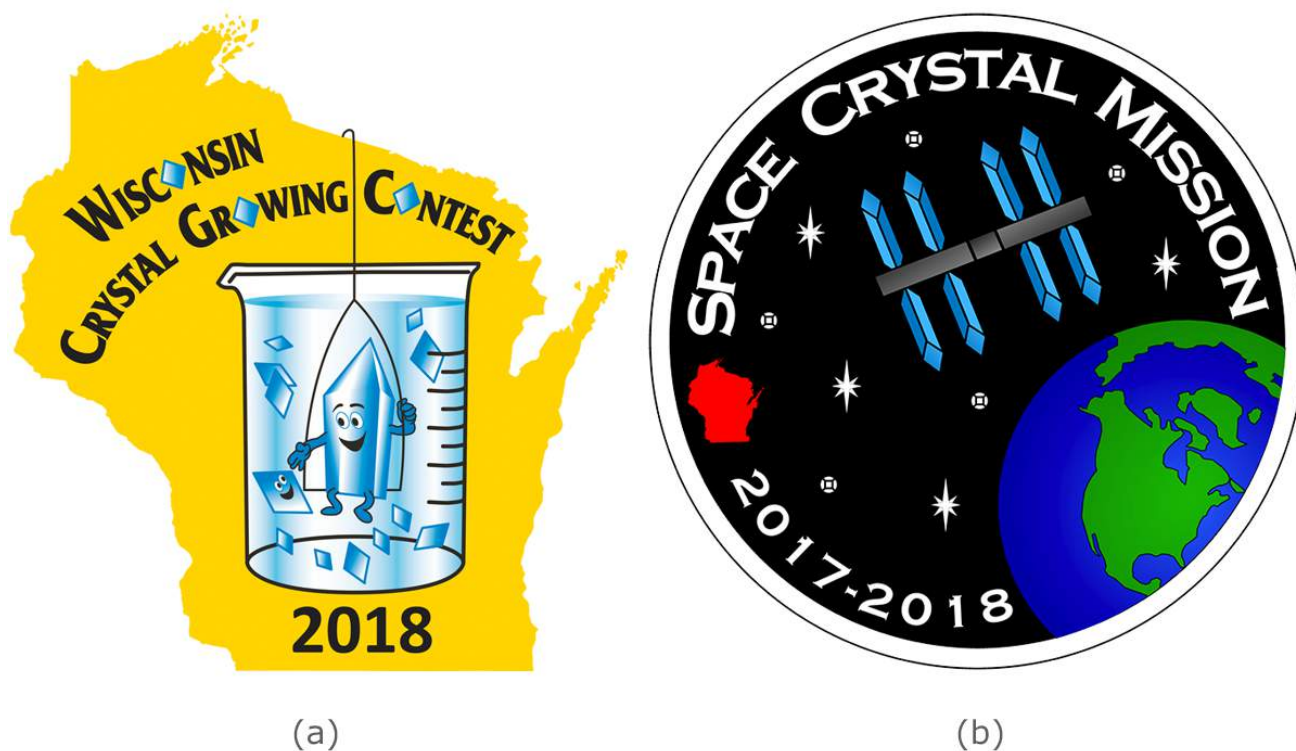


Figure 1. (a) The WICGC logo. (b) The WI Space Crystal Mission logo designed by the student art team. Earth signifies the location of the ground control experiments and the ISS signifies the location of microgravity crystallizations; the ISS solar panels are blue to reflect the color of $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$, and the white stars symbolize KDP (potassium dihydrogen phosphate). The logo could not display the US flag, but the state shape in cardinal red is Wisconsin.

In 2017 a spectacular development took place: the WICGC organizers launched a collaboration with CASIS (Center for the Advancement of Science in Space), the manager of the [International Space Station U.S. National Laboratory](#) (ISS NL). As a result, the winners of the 2017 and 2018 WICGCs were privileged to collaborate with CASIS scientists and have the singular experience of conducting crystallization experiments aboard the ISS!

The winners of the top six prizes in the 2017 WICGC were offered the chance to collaborate on the Space Crystal Mission and boy, did they hit the jackpot! The program exposed the students to the special characteristics of engineering, research and operations in a space environment. The students had to translate and optimize ground laboratory experiments to spaceflight conditions aboard the ISS NL. Scientists from University of Wisconsin-Madison, Covance Clinical Research Unit and CASIS guided and educated the students through all phases of the project; however, the students (ages 11-18) were treated as adults and had to perform all the work themselves (Figure 2). Participants' efforts were fruitful and at the end of this 10-month endeavor the students successfully obtained crystals of $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$ and KDP aboard the ISS NL in specially designed flexible transparent containers by the thermal gradient technique. The crystals were expected to be of higher quality than on Earth due to the diffusion-controlled crystallization dynamics in the absence of convection and sedimentation.

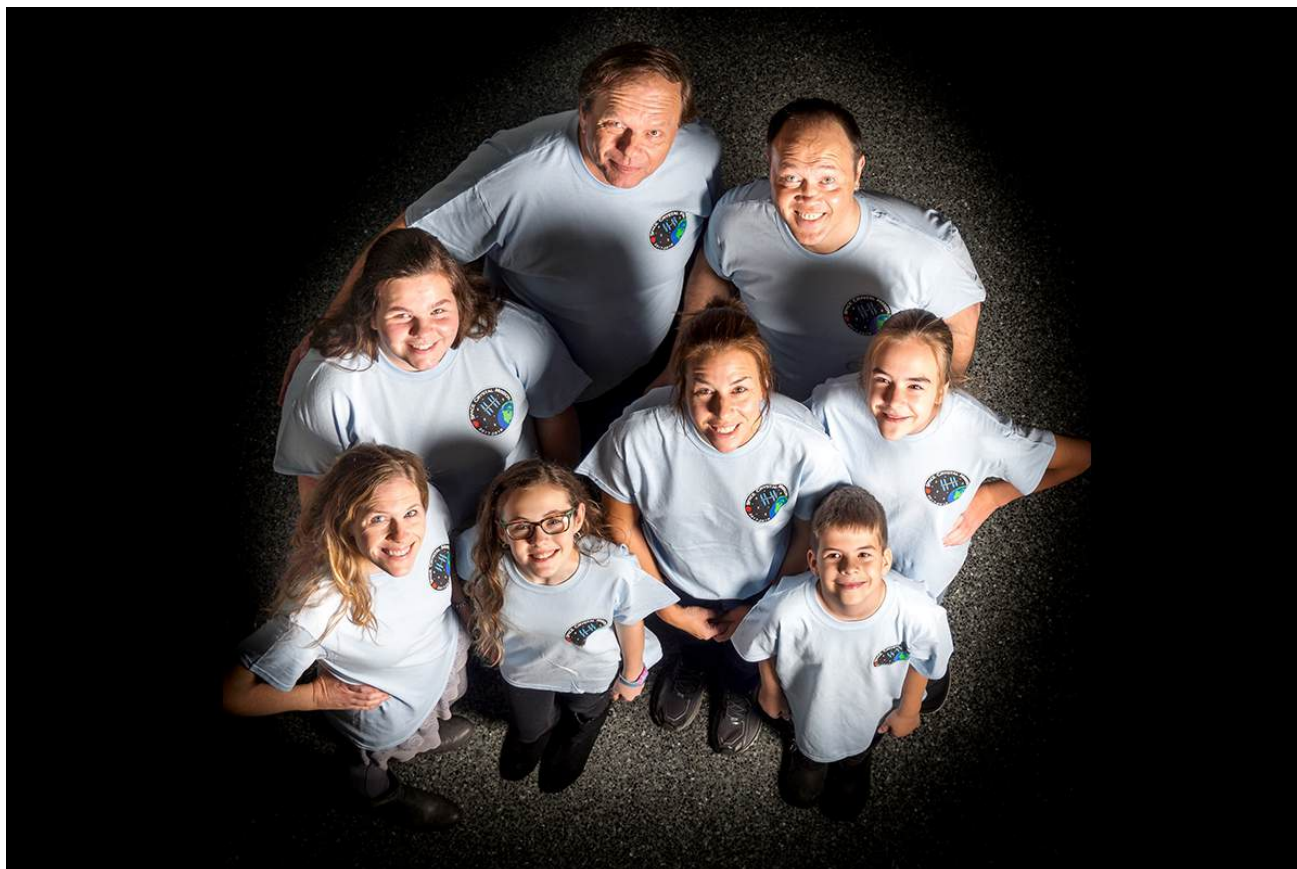


Figure 2. WI Space Crystal Mission participants and their family members viewed from the perspective of the ISS.

The Space Crystal Mission was educational for the team leaders, but it is the benefits to the students that must be particularly stressed, because nobody is better at outreach than CASIS and the National Aeronautics and Space Administration (NASA). The winners of both the crystal growing contest and the art contest were invited to participate by CASIS. The project began in May 2017 with a visit by a CASIS senior research scientist Marc Giulianotti. In August 2017, a payload specialist April Spinale from CASIS visited Madison to give a lecture to the students and their parents about the experiment design and the eventual visit to Cape Canaveral. By November 2017, all hardware had been designed and ground control experiments conducted. In the process the students learned to collaborate remotely with their peers and leaders, write professional e-mail messages, prepare posters and PowerPoint presentations, critique each other's work, take laboratory notes and use new software programs.

We arrived in Cape Canaveral four days before the launch on March 29, 2018, and took the afternoon to familiarize ourselves with the wet lab at the CASIS Space Life Sciences Building. On March 30 the students prepared the solutions and charged the crystallization apparatuses with crystallization materials. Dr Zoran Radić (University of California, San Diego, USA) set up a virtual reality exhibit for the students to explore proteins and take a virtual selfie (see beginning of the article)! On March 31 the leaders turned over the experiments (which were not to be touched with bare hands) to NASA specialists who verified the contents and then weighed, measured, photographed and documented the submission. The hard part was over, and the fun began. On April 2 the team arrived at the Kennedy Space Center where the students gave a short oral presentation at the Journey to Mars pavilion along with other student teams. At 16:30:38 we gathered at the VIP viewing area and watched the SpaceX CRS-14 Dragon capsule with a Falcon 9 booster launch to the ISS; the live commentary from the control center over loudspeakers was outstanding. It was extremely satisfying to witness the take-off, watch the rocket disappear into the sky, and follow the flight progression via a live feed from the cameras on the rocket. A few minutes into the flight, the solar panels unfolded and the Earth entered the background - a sight our

team will never forget. After high-fiving, there was more work to do - the students had to present posters to the public in the Apollo/Saturn V pavilion under the rocket.

Two members of our team were later selected by CASIS to participate in the ISS R&D conference in San Francisco in July 2018 (all expenses paid). Among the typical conference activities, this engagement required Kaitlyn Twesme (14 years old) and Payton Kelly-Van Domelen (13 years old) to serve as panelists with a peer student group in a large auditorium in front of several hundred people. During this round-table event there was a live downlink from the ISS, and American astronaut Andrew Feustel answered a question from each of the 10 students! Through all stages of the Space Crystal Mission the students gave presentations at schools, libraries and chemistry departments, and even appeared on local TV. I have kept in touch with the students after the space crystal project and can attest that they have grown into independent and motivated individuals with leadership qualities. It was certainly a lot of work for the students (the parents know!) but they benefitted in ways that we did not originally envision.

The popular WICGC took off (pun intended) in a different direction in 2017 and we expect to attract even more participants in the future.

OUTREACH

A diamond is not forever: crystals and changes at the Science Festival in Genoa, Italy

Alessia Bacchi



Boards showing the contrast between mystic Hildegard von Bingen and scientist Dorothy Hodgkin (left) and the metamorphosis of calcium carbonate from shell to statue (right).

The theme for the Science Festival in Genoa this year was 'Changes'. That is quite challenging for those who study crystals, which are normally considered symbols of eternity (diamonds are forever, we are used to hearing). But crystallographers love challenges, and we organized the exhibition 'Crystals and metamorphosis', showing the beauty of phase transitions, polymorphism and metamorphism. Visitors enjoyed discovering the several forms of ice, the scary instability of diamonds contrasted with graphite ("I will bring you a pencil for our next anniversary" said a boy to his girlfriend), the transformations of calcium carbonate from shells to Michelangelo's David, the story of tin pest, of chocolate bloom, and also the discovery that drugs may be polymorphic. The graphic layout was designed to highlight the idea of change between contrasting concepts. Along with crystal transformations, another kind of dualism was presented for people's meditation: crystals between science and magic, and vision between science and literature. In the former, Hildegard von Bingen and Dorothy Hodgkin were paired to show the contrast between a mystical view of the universe and a scientific approach leading to discovery; in the latter, the vision of the structure of benzene by Kathleen Lonsdale and the beauty of the structure of lonsdaleite were paired with the fantastic descriptions created by Italo Calvino in imagining the birth of crystals in a primordial world.

The exhibition was open between 25 October and 5 November 2018 at the Museo del Mare Galata in Genoa, and was organized by Alessia Bacchi and Paolo Mazzeo of the University of Parma (Dipartimento SCVSA and Sistema Museale di Ateneo), with graphic design by Valentina Manente and with the sponsorship of the Italian Crystallographic Association. The exhibition was supported by the IUCr and by the ECA.

Visitors were invited to write impressions and graffiti on two boards before leaving: we collected lots of hearts and diamonds; maybe some future Dorothys left their name here.

OUTREACH

Who can be a crystallographer?

Claire Murray



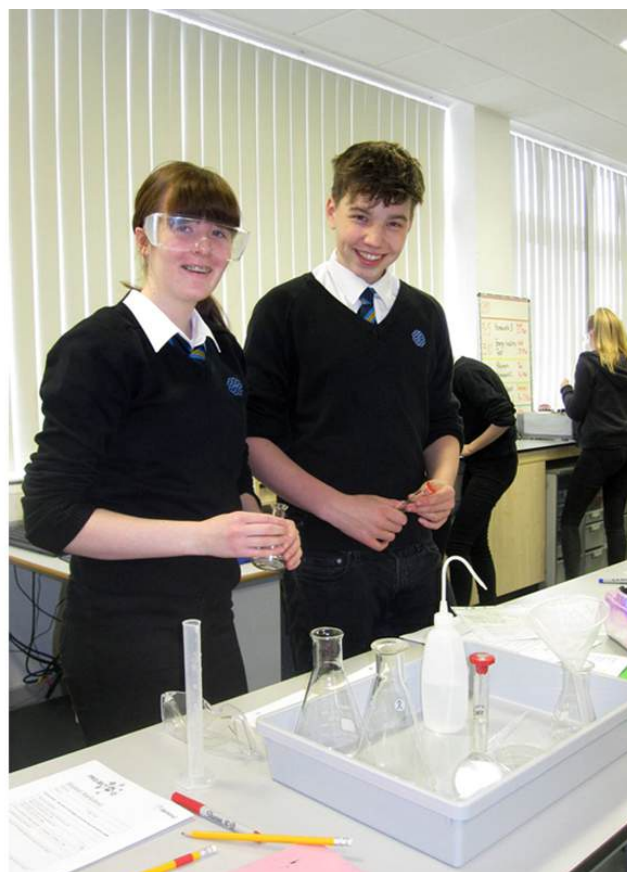
For those of us who have been through years of learning and training, it seems somewhat strange to answer this question with “anyone”. The incredible depth of our field and complexity of our science have bewitched so many of us, that jumping feet first into being a crystallographer with no professional experience seems impossible. But we should remember that people can contribute to science in different ways and at different levels. Thinking outside the box, we have the tools and the knowledge to share the fundamentals of crystallography to, in turn, empower people to participate in crystallography in whatever way they can. This is the fundamental goal that underpins the biggest ever outreach project at Diamond Light Source, Project M.

Student participation in real science is an idea that many people have been exploring, including [Zooniverse](#) and the [Institute for Research in Schools](#) to name two of many. Given the speed, power and knowledge at a synchrotron, experiments that engage lots of students would absolutely be something we could excel at. Enter [Project M](#) (Twitter: [@DLSProjectM](#)), where over 1000 students from 100 schools all over the UK participated in 1 experiment running over 24 hours at Diamond Light Source on Beamline I11, the high-resolution powder diffraction beamline. Beamline I11 has a robot and sample carousel that can hold 300 samples, so this was the perfect starting place for this project.

The most critical question for this project, however, was what scientific question could the students help us answer? Calcium carbonate is the most abundant biomineral, being produced by organisms for use as shells, skeletal supports and even optical lenses. The ability of nature to direct CaCO_3 crystallisation is frequently explored through biomimetics, whereby the addition of reagents that mimic the biological

scaffold influence CaCO_3 formation. Amino acids are the simplest descriptor of the biological scaffold, being an analogue of the protein side chains observed in biomineral organic matrices. Our group had studied the synthesis of calcium carbonate with amino acids previously and it turns out that calcium carbonate was conveniently already on all of the UK curricula, which meant it would tie in with the teachers' learning objectives for the students. The synthesis of this material is also already performed in secondary school labs and the safety hazards attached are very low. By providing each school with a different amino acid to act as a scaffold for directing crystallisation, the students could explore the impact of increasing concentration of amino acids on polymorph formation and on lattice expansion due to incorporation. The large number of participants would enable the screening of a large number of amino acids.

The logistics of delivering such an experiment are really not trivial. Even the act of packing up boxes to send to schools required huge planning and a team of over 30 people who helped throughout the day to make the boxes, sort the paperwork and ensure each box had everything it needed before sending them off. Investment into resource development and testing was also essential - the instructions and methodology chosen had to work in secondary school labs. It is very easy to forget that secondary school students do not have access to the same equipment or knowledge of language that we do!



The project took over 2 years to develop but it only required 24 hours of beamtime. The day itself was full of excitement and anticipation, with a live video of the experiment throughout the process so everyone could see the robot mounting samples and the detectors moving. The data were also live tweeted so that the schools were able to see their diffraction patterns (Twitter: [@DLSProjectMLive](#)). Following the experiment, the data were all uploaded to a website where the students could interact with their data. Tools were specially built to facilitate peak fitting and comparison of diffraction data with standards and with other similar data and so students could work out which polymorphs they had made and compare with other student data for similar samples.

The response to this project has demonstrated that there is a real appetite for teachers and students to engage with real science and we would strongly encourage you to give it a go. It is a lot of work to

undertake, but the rewards in knowing that students have an opportunity to learn about and participate in real science are tremendous. We were also very excited when we started analysing the data as there were some fantastic results. The volume of data does limit the rate of progress, but we are in the process of preparing a manuscript and hope to publish the data soon. This project would not have been possible without a huge team of internal and external people who contributed in so many ways, and we are all incredibly grateful to everyone for helping to make this happen.

SPECIAL REPORT

Sharing structural data

Suzanna WardFrancesca Stanzione



ICSD Entry: 239053

[Sign In](#)
 Licensed to: CCDC Main Site

[Simple Search](#)
[Structure Search](#)
[Unit Cell Search](#)
[Formula Search](#)

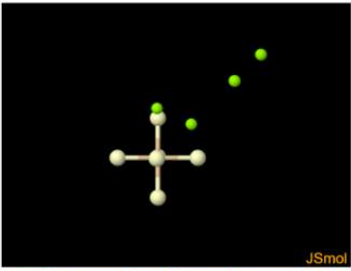
Your query was: DOI: 10.1021/acs.inorgchem.5b02114 and the search returned 14 records. [Modify Search](#) [New Search](#)

Database Identifier	Deposition Number
☒ ICSD 239052	1485056
☒ ICSD 239053	1485057
☒ ICSD 239054	1485058
☒ ICSD 239055	1485059
☒ ICSD 239056	1485060
☒ ICSD 239057	1485061
☒ ICSD 239058	1485062
☒ ICSD 239059	1485063
☒ ICSD 239060	1485064
☒ ICSD 239061	1485065
☒ ICSD 239048	1485066
☒ ICSD 239049	1485067
☒ ICSD 239050	1485068
☒ ICSD 239051	1485069

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ICSD 239053 : ICSD Structure : $\text{Ce}_9\text{Si}^{10-23}(\text{Mg}^{2+})$
 Space Group: $Fm\bar{3}m$ (225), Cell: $a\ 14.586(9)\text{\AA}$ $b\ 14.586(9)\text{\AA}$ $c\ 14.586(9)\text{\AA}$ $\alpha\ 90.00000^\circ$ $\beta\ 90.00000^\circ$ $\gamma\ 90.00000^\circ$

3D viewer



[H](#)
[Disorder](#)
[Labels](#)
[Menu](#)
[Open](#)

Style: [Ball and Stick](#)
 Labels: [No Labels](#)
 Packing: [None](#)

Measure: [None](#)

Chemical diagram

More Information Available from the ICSD
http://www2.fiz-karlsruhe.de/icsd_home.html

[View group symbols key](#)

Additional details

Deposition Number	1485057
Deposited on	13/06/2016

The crystallographic community is remarkable in terms of its data-sharing practices, which allow scientists worldwide to gain new insights and knowledge from the collaborative collection of data. These exemplary data-sharing practices have enabled a number of crystallographic databases to exist for over 50 years and researchers have been able to learn from comprehensive archives of crystal structures covering inorganic, organic, metal-organic and biological macromolecular compounds, which has been of enormous value to a wide range of research applications. In crystallography, however, there isn't just one database but a variety of different ones, differing in subject area or chemical space, experimental or computational method and database implementation, sustainability and access models. Clear distinctions were drawn up between some databases when they were established and researchers needed to know into which database to deposit their data and which database to search for their particular subject area. In the decades since these databases were set up the world has changed, as have the needs and expectations of the researcher. Advances in science mean that the distinctions between historically separate disciplines and sectors have become blurred; for instance, in research to design new batteries, gas storage systems, zeolites, catalysts, magnets and fuel additives all cross the boundaries between the worlds of inorganic and organic structures. This is coupled with a desire from researchers for more integrated databases and the expectation that a single search will be able to find all the required information.

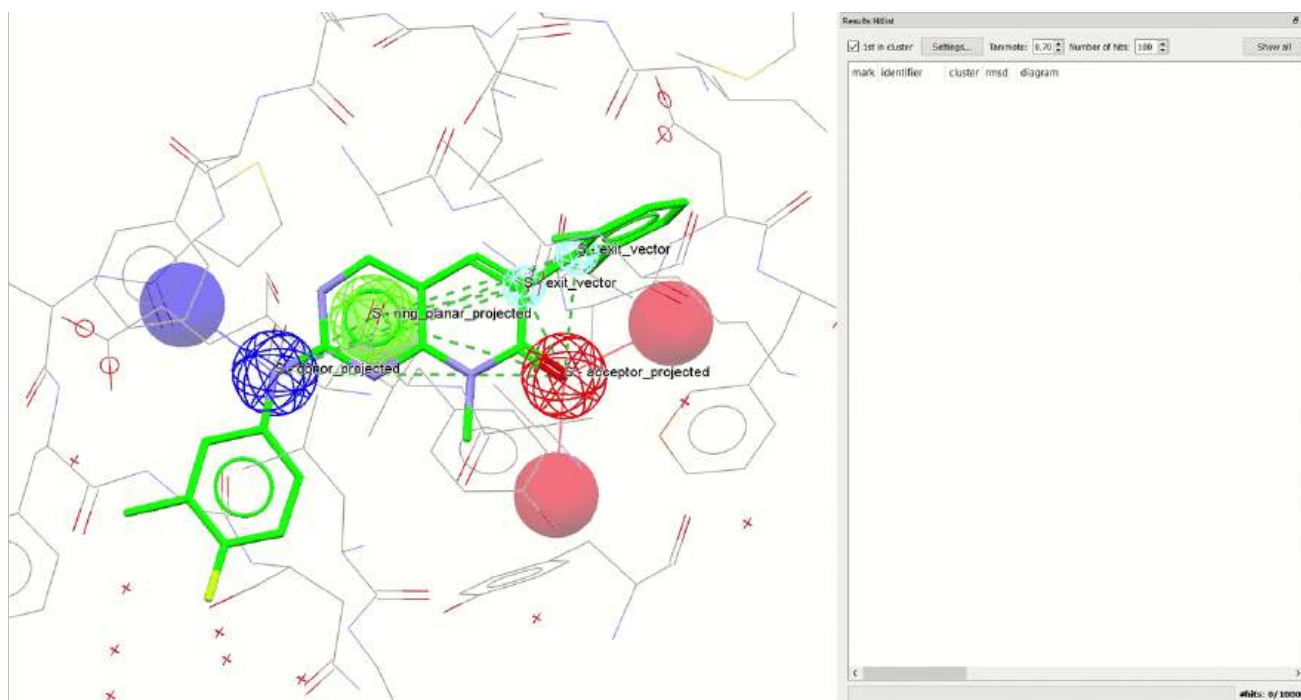
Over the last few decades these desires and expectations have led to more collaborations, integrations and linking between data sources, be it publishers and repositories or between the data repositories

themselves. The Cambridge Crystallographic Data Centre (CCDC) is one of many organisations that has started to adapt to these changing landscapes.

Earlier this year we saw the launch of joint deposition and access services for crystallographic data across all chemistry through a collaboration between the CCDC and FIZ Karlsruhe – Leibniz Institute for Information Infrastructure (FIZ Karlsruhe). As a result, researchers and educators worldwide, working across all fields of chemistry, are now able to explore over one million crystallographic structures through a joint Access Structures service, enabling them to view and retrieve deposited data sets associated with structures in the Cambridge Structural Database (CSD) and the Inorganic Crystal Structure Database (ICSD). This was the result of a large-scale project to unify deposition and access processes at the CCDC and FIZ Karlsruhe, and both organisations are agreed on the value this has for the community and look forward to collaborating further in the years to come.^[1]



In parallel with this work the CCDC has been working closely with the Protein Data Bank (PDB) and these close ties have resulted in a variety of joint activities. An example is the integration of *Mogul* into the PDB's ligand validation pipeline for newly deposited structures, which allows researchers to use the knowledge-based library of molecular geometry derived from the CSD to check the geometry of their ligands. Three years ago we also saw the introduction of linking between the PDB's chemical component dictionary and structures in the CSD to allow researchers to more easily connect between the two data resources. More recently the CCDC has also developed *CSD-CrossMiner*^[2] to allow users to search databases such as the CSD and the PDB simultaneously using pharmacophore queries. This delivers an overall interactive search experience with application areas in interaction searching, scaffold hopping or the identification of novel fragments for specific protein environments.^[3] While developed from a drug discovery perspective, these methods are potentially applicable in broader fields, for example to find potential co-former molecules for crystallisation or for finding promising new ligating moieties in organometallic compound design.



An animation of *CSD-CrossMiner*: dynamic 3D pharmacophore searching across the CSD and the PDB. Matching hits and their 2D diagrams are displayed on-the-fly providing an interactive search experience.

We hope that these community initiatives are of value to researchers worldwide and we look forward to being driven towards new opportunities and collaborations based on the needs of the community we serve.

[1] <https://www.ccdc.cam.ac.uk/News/List/2018-07-new-joint-services/>

[2] <https://www.ccdc.cam.ac.uk/solutions/csd-discovery/Components/CSD-CrossMiner/>

[3] *Interactive and Versatile Navigation of Structural Databases*, O. Korb, B. Kuhn, J. Hert, N. Taylor, J. Cole, C. Groom and M. Stahl (2016). *J. Med. Chem.* **59**, 4257-4266; DOI: [10.1021/acs.jmedchem.5b01756](https://doi.org/10.1021/acs.jmedchem.5b01756)

MEETING REPORT (IUCR SUPPORTED)

RapiData 2018

Silvia RussiClyde SmithAna Gonzalez



RapiData 2018 participants.

The RapiData 2018 practical workshop in macromolecular X-ray crystallography was hosted by the Structural Molecular Biology (SMB) group at the Stanford Synchrotron Radiation Lightsource (SSRL) in Menlo Park, CA, USA, from 22 to 27 April 2018. As in past editions of the course, our aim was to educate and train young scientists in data collection and processing methods at synchrotron beamlines, using state-of-the-art software and instrumentation. The co-organizers of the 2018 course were SSRL scientists Clyde Smith, Silvia Russi and Ana Gonzalez.

The 2018 course attracted 41 young and early-career scientists, mainly postgraduate students and postdoctoral researchers, but also some master students, research staff and junior faculty from around the world. One important mandate for all the previous RapiData courses has been to encourage attendance by young scientists from Latin America with the assistance of scholarships from the IUCr. As always, this IUCr support is critical, as the amount of funding available to research institutions in Latin America for student travel grants has severely diminished over the years. Moreover, as with last year, we have had to substantially increase the size of the awards in order to facilitate attendance of participants from this region. We awarded five scholarships to pay for accommodation and/or travel and subsistence expenses to attend RapiData 2018. The recipients were selected based on a letter of recommendation by their supervisor stating how the student would benefit from attending the course and how their attendance will allow for the dissemination of the practices taught at the course in their home laboratories. The awards were presented during a ceremony on the last day of the course.

On Sunday 22 April, Bob Sweet (Brookhaven National Laboratory) gave a five-hour lecture course on the fundamentals of crystallography to ensure that students without much previous experience in crystallography benefit fully from the lectures and practicals during the rest of the course. As has been the norm for the previous few years, almost all of the participants take advantage of this day of lectures. On the Monday and Tuesday there were lectures covering topics ranging from light sources, beamline instrumentation, sample preparation, data collection, indexing, integration, phasing and complementary techniques. Invited speakers were Aina Cohen (SSRL), Raji Edayathumangalam (Columbia University), Elspeth Garman (Oxford University), Andreas Foerster (Dectris), Ana Gonzalez (SSRL), Jim Pflugrath (Rigaku), Harry Powell (Diamond Light Source), Enrique Rudiño-Piñera (UNAM), Nick Sauter (LBNL), Ivan Shablin (University of South Carolina), Clyde Smith (SSRL), Bob Sweet (BNL), Tom Terwilliger (LANL) and Thomas Weiss (SSRL). Participants were also able to tour the serial femtocrystallography facilities at the Linear Coherent Light Source (LCLS). From Tuesday evening through to Thursday evening, the participants were involved in hands-on software tutorials on data reduction (*XDS*, *HKL2000*, *DIALS*) and structure solving software (*CCP4*, *Phenix*, *HKL-3000*), along with sample preparation and data collection tutorials at four SSRL beamlines. These tutorials were run by the speakers and additional tutors from the *Phenix* group (Pavel Afonine, Li Wei Hung, Nigel Moriarty, Dorothee Liebschner), *CCP4* (Andrey Lebedev) and SSRL and Stanford University staff (James Holton, Tzanko Doukov, Irimpan Mathews, Daniel Fernandez, Thomas Lane, Silvia Russi and Clyde Smith). Students were encouraged to bring their own specimens and data for data collection and processing; samples were also provided by the organizers for students who did not have their own. The course ended on Friday 27 April with an award ceremony and round table feedback meeting. Both students and speakers and tutors expressed a high degree of satisfaction with the course. Based on the positive feedback, we intend to hold the course at SSRL from 5 to 10 May 2019. See more information [here](#).

MEETING REPORT (IUCR SUPPORTED)

Sixth International School of Crystallization



A group of students and teachers inside the Alhambra Palaces.

The 6th International School of Crystallization: Drugs, Foods, Agrochemicals, Minerals, New Materials (ISC2018) took place from 20 to 25 May in the centre of the beautiful city of Granada, Spain, an ideal place to promote close scientific and social interactions between the attendees. The school was organised by the Laboratory of Crystallographic Studies (CSIC-UGR) under the auspices of the IUCr through the Crystal Growth and Characterization of Materials Commission and the Teaching Commission, with the support of the International Doctoral Summer School Programme of the School of Science, Technology and Engineering of the University of Granada, the Spanish Specialized Group of Crystallography and Crystal Growth (GE3C) and the Excellence Network of Crystallography and Crystallization “Factoría de Cristalización”. The School gathered postgraduate/postdoctoral students as well as research scientists from industry and academia that deal routinely with crystallization processes but seek fundamental knowledge on the crystallization phenomena and the behaviour of crystallizing solutions. Students from all over the world were invited to learn from top quality international speakers, to hear case study presentations, to watch practical hands-on demonstrations and to present their research results in the purposely dedicated poster sessions.

Attendance

The turnout of the School was excellent with 104 participants from 17 countries, including 50 students. Considerable effort was made to provide financial support to as many students as possible; in fact, all

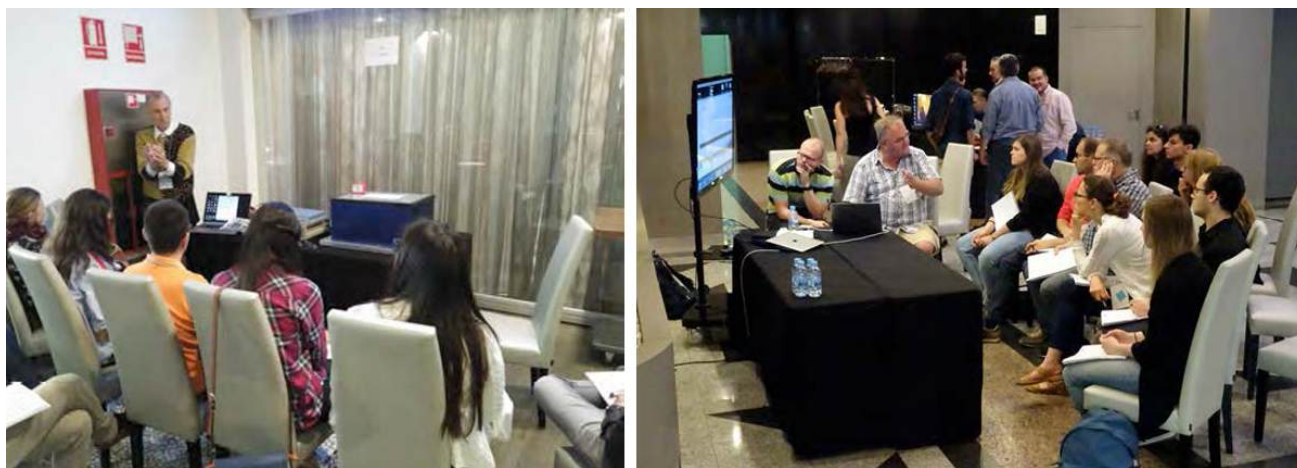
grant applications were accepted for funding. Remarkably, most of the granted students came from outside Spain.

Programme

ISC2018 covered five days of lectures and practical demonstrations carried out by 29 selected experts in fields directly related to crystallization. The main topics were solution properties, nucleation: classical and non-classical approaches, crystal growth kinetics and mechanisms, crystallization routes, crystallization techniques, crystal morphology, mineral textures, polymorphism, hydrates and solvates, crystallization screening, industrial (mass) crystallization, crystallization in microfluidics, chirality, biomineralization, mesocrystals, nanocrystals and co-crystals.

The first day of the School dealt with the fundamentals of crystallization from solution encompassing a revision structure and properties of crystallizing solutions, nucleation theories, crystal growth kinetics and mechanisms, morphology and structural defects. The second day of the School focused on both classical and novel crystallization techniques including solution vs. gel growth, crystallization from melts and crystallization in microfluidic systems. There were also lectures on hollow crystals, mesocrystals and nanocrystallization. On Wednesday there were two markedly different sessions on special topics. While the morning session was devoted to discussing the fundamentals of polymorphism, co-crystallization and chiral crystallization, the afternoon was dedicated to biological crystallization. In the evening, Juan Manuel García-Ruiz gave a special talk on the symmetry of the Alhambra, which was followed by a night visit to the Alhambra Palaces.

Thursday was entirely dedicated to a 'Demonstrations Fair', at which 18 specialists offered short (20-40 minutes) practical sessions periodically at scheduled times. Participants could choose what sessions they wanted to attend and in the order they wished, so that they selected their own learning programme "à la carte". The Demonstrations Fair proved to be an excellent teaching tool as it provided students with plenty of opportunities to interact on a personal basis with tutors and to watch closely how to perform crystallization experiments.



Demonstration Fair: Left: Jörg Hulliger explaining crystal growth equipment for controlled growth from solution: temperature difference and evaporation technique. Right: Helmut Cölfen and Denis Gebauer explaining how to analyse prenucleation clusters and synthesize mesocrystals.

On the last day there were lectures on special hot topics, including crystal engineering of task-specific materials, mineral assembly and analysis of the structural organization of mineralized tissues. In addition, there was a round table on "Classical vs. non-classical nucleation", one of the most debated topics in crystallization nowadays. The round table was moderated by Lourdes Fernández Díaz, and featured Jim de Yoreo, Denis Gebauer, Christine Putnis and Giuseppe Falini.

The School closed with the presentation of poster prizes offered by the IUCr and the Crystallization Factory of the Laboratory of Crystallographic Studies.

Poster Sessions

Dynamic and lively poster sessions rounded off each day and proved to be a very valuable opportunity to discuss the scientific work. Students made a great contribution by presenting 44 posters. An international panel of lecturers decided to award five prizes for the best poster presentations. The two IUCr prizes went to Hans Hendrikse (AMOLF, the Netherlands) and Francesca Carella (Istec-CNR, Italy) while the three Crystallization Factory prizes were awarded to Panayiotis Klitou (University of Leeds, UK), Cristina Ruiz-Agudo (University of Konstanz, Germany) and Fabian Kurzeman (University of Innsbruck, Austria).

Social events

In addition to the scientific course, there was a parallel social programme, which consisted of a welcome cocktail on Sunday, a night tour of the Nazaries Palaces of The Alhambra on Wednesday and a Flamenco dinner party on Thursday in the Carmen de la Victoria in the Albayzin district.

Evaluation

Overall, the School was deemed to be very successful as judged by the majority of positive comments written in the evaluation form by the participants. The attendees were asked about three major items: the quality of the scientific programme, the Demonstrations Fair and the organisation.

Conclusions

According to the evaluation forms, the school was considered very valuable by the participants, partly because of the quality of the programme and partly due to the contribution of some of the best lecturers for the wide range of topics covered. All in all, the ISC2018 was an enriching experience for all of those involved, triggering several fruitful scientific discussions. The positive approach, the openness and the active participation of each of the participants made it a wonderful experience, worthy of being repeated in the future. We would like to express our gratitude to all of the participants; to the teachers for their full commitment and to the students and colleagues from academic and industrial backgrounds for believing in these Crystallisation Schools. We are very grateful to all the people who have worked very hard in preparing the Schools to make them successful. Last but not least, we would also like to express our gratitude to the sponsors and exhibitors for their great support.

A full report of the meeting is available [here](#).

MEETING REPORT (IUCR SUPPORTED)

International School of Crystallography 52nd Course - Quantum Crystallography

Annalisa Guerri



The 52nd Course of Crystallography at the Ettore Majorana Research Foundation in Erice, Italy, coincided with the inaugural school on Quantum Crystallography, and took place from 1 to 10 June 2018. The course ran in parallel with the 51st Course on Electron Crystallography.

A total of 56 students from 16 countries and 25 lecturers/tutors attended the school, filling all the seats available.

The lectures started with fundamentals of crystallography (symmetry, diffraction, modelling) and quantum mechanics (the Schrödinger equation, wavefunctions, physical bases of the models). The lectures then focused on the most adopted methodologies (experimental as well as computational) to determine the charge and spin electron density, the wavefunction and the electric and magnetic properties of crystalline materials. In the last sessions of the meetings, the lecturers presented applications of quantum crystallographic studies. A round table concluded the meeting, reviewing some topics discussed with an outlook on open questions and future studies. During the 5 tutorial sessions, 10 workshops were organized based on the most broadly adopted and updated programs for multipolar models, X-ray constrained wavefunctions, periodic wavefunctions and electric/magnetic properties.

During each lecture session, a sufficient amount of time was allocated for discussion and questions from the students, who interacted quite intensively with the lecturers. The students also demonstrated interest outside the official sessions, during the breaks or social activities.

As usual at the Erice meetings, the social program was extremely rich and pleasant, including social dinners and a get-together party, music events and excursions to historical sites in the neighborhood. The participants appreciated these activities and also took advantage of the opportunities for extra discussion sessions, in an informal fashion and more relaxed atmosphere.

During the closing ceremony on the last day of the school, several prizes were awarded to students: best poster prizes and the Lodovico Prize, which is awarded to the student who has been the most lively participant, both inside and outside the lecture hall. The third place for the poster prize was awarded to Alexey Kuzmin, PhD student at the Institute of Solid State Physics, Russian Academy of Sciences (RU); the award for second place was assigned to Alena Vishina, Postdoc at the Chemistry Department, Chalmers University of Technology (SE); and first place was awarded to Emil Damgaard-Møller, PhD student at the Center for Materials Crystallography (CMC), Aarhus University (DK). The committee decided to award the Lodovico Prize to Lorraine Andrade-Malaspina, PhD student at the University of Bremen (DE).

At the end of the course, the participants received an electronic survey to evaluate and comment on the quality of the program. Their responses indicated that a similar meeting should be held at least within 3-4 years and that the course had achieved most of its objectives (score 85/100).



Award-winning students of the two courses, directors and local organizers. From left to right: Joke Hadermann (BE), Lorraine Andrade Malaspina (DE), Emil Damgaard-Møller (DK), Paul Benjamin Klar (ES), Alexey Kuzmin (RU), Paola Spadon (IT), Alena Vishina (SE), Stefan Noisternig (A), Olga Chovnik (IL), Eu Pin Tien (UK), Andy Stewart (IR), Annalisa Guerri (IT), Dylan Jayatilaka (AUS), Piero Macchi (CH) and Lukas Palatinus (CZ).

MEETING REPORT (IUCR SUPPORTED)

4D Workshop: Deep-time Data Driven Discovery and the Evolution of Earth



One of the two poster session receptions. Photo credit: Jennifer Mays.

The [4D Workshop: Deep-time Data Driven Discovery and the Evolution of Earth](#) brought together 150 participants and observers from a variety of fields, including geology, biology, data science, modeling and visualization, and science administration, to explore the evolution of our planet and ourselves. The workshop was convened from 4 to 6 June 2018 at the historic Carnegie Institution for Science Headquarters in downtown Washington, DC, USA, and focused on the application of data-driven discovery techniques to important “big questions” in the earth and life sciences:

- What was the geological and geochemical context for life’s origins?
- Did biological catalysis follow from the chemistry of rocks and minerals?
- How did Earth’s earliest microbial life interact with and influence the geosphere?
- How did plate tectonics begin and to what extent are the Earth’s surface and deep interior linked?
- When, and at what rate, did photosynthesis modify our planet’s near-surface environment?
- How did life’s subsequent complexification and migration to land alter geological and geochemical processes?



Group photo. Photo credit: John Strom.

Each day's collaborative, interdisciplinary program included a small number of plenary talks followed by a series of breakout groups. The breakout groups targeted particular subjects in data-driven discovery, and together the participants of each group assembled a set of PowerPoint slides summarizing their discussion. Workshop organizers are using these slides, along with other input gathered at the workshop, to compose a white paper outlining needs and opportunities in data-driven discovery.

Recordings of the workshop's plenary talks, as well as breakout group PowerPoint slides, are available on the workshop website's [archive page](#).

The workshop was led by an [Organizing Committee](#), chaired by Yana Bromberg (Rutgers University) and Robert Hazen (Carnegie Institution for Science), and a [Senior Advisory Council](#), chaired by Marcia McNutt (National Academy of Sciences).

MEETING REPORT

Zurich School of Crystallography 2018 in Tianjin, China

Hans-Beat Bürgi Tony Linden



The eighth Zurich School of Crystallography (ZSC) pitched tent at Tianjin University from 17 to 28 June 2018 following an invitation by Professor Jay Siegel, Dean of the School of Pharmaceutical Science and Technology (SPST). The school was attended by 20 handpicked participants, 9 from the Tianjin area, 8 from various other parts of China, 1 from Hong Kong and 2 from Thailand. Of these, 2 are studying towards an MSc, 11 are PhD students, 2 are Postdocs and 5 are young academics. Seven of the long-time Zurich School tutors from the universities of Zurich, Bern, Prague, ETHZ and EPFL took up the invitation, namely Tony Linden, Olivier Blacque, Hans-Beat Bürgi, Lukas Palatinus, Michael Wörle, Bernd Schweizer and Gervais Chapius. Richard Cooper from Oxford University, Ian Williams from Hong Kong University of Science and Technology and Junliang Sun from Peking University completed the team, thereby ensuring our usual and popular 2:1 student:tutor ratio. The goal of the school is to equip each participant with enough theory and practice to be able to determine small-molecule organic and inorganic crystal structures and to recognize difficulties that require help from a more experienced specialist. The encounter of the mostly western teachers with the Asian students was both interesting and at times somewhat challenging, but in the end very rewarding.

The programme followed our well-tried format, usually with two hours of lectures followed by two hours of practical work during the mornings and afternoons. The participants had to solve at least three set structures and could then work on their own data set collected from a sample they provided. The specially selected set structures provide increasing levels of complexity. The first one is straightforward

and allows the participants to learn the general procedure from structure solution through to a completed and validated structure report using the program package *Olex*². The second one requires some chemical knowledge for proper atom assignment, while for the third one the chemist's guess of the structure is largely wrong and the actual molecular structure has to be found using a combination of chemical, crystallographic and geometrical logic and even databases. Examples involving severe disorder and solvent molecule handling were also demonstrated.

The SPST is well equipped with three recently installed Rigaku diffractometers: a Synergy-S and a XtaLAB Synergy Custom FR-X Rotating Anode system with two ports. In addition, we had access to a Rigaku SuperNova diffractometer at the School of Science, Tianjin University, thereby allowing the participants adequate opportunity to gain hands on experience with data collection procedures using their own samples. Yan Zier from Rigaku China was on hand to assist with the brand new instruments and his expertise was highly appreciated. Structure solution, refinement and analyses were done in a fully equipped computer room, which provided a workstation for each participant and tutor.



We found that the student-tutor interaction in China is somewhat more reserved than what we are used to in Zurich and this was particularly noticeable during the lectures. Although the participants spoke good English, their pronunciation sometimes needed getting used to. We also learned that the Chinese language has technical terms that are very different from the English ones and it was here that the help of our Chinese colleague Junliang Sun was invaluable, as he usually untangled communicative roadblocks with a single, short sentence in Chinese. Some of the lecturers felt at times that their message did not get through, but as the school proceeded it became increasingly clear that the participants understood enough of the lectures to be able to consult their Chinese text books and discuss the day's material together at the hotel in the evening. Thanks to the 2:1 format during the practical work, the interaction between the participants and the tutors became increasingly more relaxed. The very successful outcome of the final two-hour written exam showed how really hardworking everybody was. When Lukas Palatinus from Prague started playing the guitar after the final dinner, everybody joined into the singing and the two cultures had definitely merged into a single, merry group.

On the rest day, the tutors were taken to the Huangyaguan Pass section of the Great Wall and almost had the wall to themselves during the strenuous 2.2 km walk along the ridge and down to the river. It was a great experience.



Professors Jay Siegel, Kim Baldridge and SPST made an enormous effort to provide a congenial atmosphere for the school and excellent accommodation. We are especially grateful to Jun Xu who did most of the local organization, including initial data collections and structure solving for the crystalline samples contributed by the participants, thereby ensuring that they did not have to work on didactically unsuitable structures. Without the efforts of Ying Wei, the Europe-China communication, transportation and visa arrangements would have been significantly more difficult. Vice Dean Zhou Yan acted as the local coordinator and organizer. The directors and local organisers very much appreciate the willingness of the tutors to undertake this adventure. Tianjin University, The Health Sciences Platform of Tianjin University and Rigaku Oxford Diffraction supported the school financially. We also wish to thank the Cambridge Crystallographic Data Centre and the Fachinformationszentrum Karlsruhe for permission to access their databases during the school, plus the IUCr for access to [International Tables Online](#). Last but not least, the tutors are very grateful to the volunteer students who accompanied them between the hotel and the university and made sure that we did not get into difficulties in a country where we knew only a handful of words. Xiè xiè!

Report from a participant

The Zürich School of Crystallography (ZSC), 2018 in Tianjin was a great surprise for Chinese scholars. I would say joining this school is one of the best things I've ever done. I can feel how considerate ZSC is. We had a Chinese tutor this year for dealing with language issues, which turned out to be a very wise and helpful decision.

The tutors were kind, patient and knowledgeable. What impressed me most was their open-mindedness and enthusiasm towards a new culture. They adapted themselves very quickly to China's environment by learning Mandarin and gestures, using WeChat and climbing the Great Wall in Tianjin.



Mengsi Lu.

Another thing to be mentioned is the 2:1 student:tutor combination, which is the most beneficial and effective part of this course. Chinese students tend to keep quiet in discussions, which may be inefficient for feedback and interactions. But within a small group, I felt free to ask whatever I wanted. Meanwhile, my tutor would try his best to answer my questions, no matter how trivial or how strange they were.

The ZCS covered everything I could imagine about crystallography, from fundamental backgrounds to the practical operation of solving structures, including the introduction of instruments and the output of the final report. No wonder how intense it is! Fortunately, the theoretical concepts were repeatedly taught during the whole course and externalized in practical session. I have a systematical map in my mind with more confidence and ability to work on crystals after the school.

I had a great time during the school, where I met many people from around China and made two friends from Thailand. The final banquet was full of joy and music; I enjoyed it very much.

In the end, I appreciated everyone who contributed to this school and made it so successful and meaningful. I strongly recommend ZCS to anyone who is interested in this area. This will be a good opportunity to immerse yourself in the ocean of knowledge.

Mengsi Lu, Tianjin University, China

If you are interested in the next Zürich School of Crystallography, which will take place at the University of Zürich, Switzerland, from 16 to 27 June 2019, please go [here](#).

MEETING REPORT (IUCR SUPPORTED)

Fifth European Crystallographic School

Catharine EsterhuysenDelia A. Haynes



Excursion dinner at Spice Route wine estate.

The Fifth European Crystallographic School (ECS5) was held under the auspices of the ECA, the IUCr and the South African Crystallographic Society (SACrS) in Stellenbosch, South Africa, from 8 to 14 July 2018. The school was attended by 86 participants, including 21 lecturers and tutors, from 13 different countries, primarily from Africa. The first part of the school, from 8 to 10 July, constituted an introduction to the fundamentals of crystallography, including symmetry, space groups, diffraction physics, crystallization and the theory behind data collection, structure solution and refinement. From 11 to 13 July the participants divided into two groups, one focusing on materials science and the other on structural biology.



Ilia Guzei explaining diffraction geometry.

The structural biology session included a visit to the University of Cape Town for a demonstration of the instrumentation housed in the Structural Biology group, as well as hands-on sessions on crystallization and structure solution and refinement. The materials science grouping also focused on hands-on sessions, covering topics such as the Cambridge Structural Database, structure solution and refinement, powder diffraction (including Rietveld refinement) and solution of twinned and disordered structures. There was also a demonstration of the Stellenbosch University diffraction equipment. On the final day of the school the two groups joined up again for a description of how to report crystallographic data, neutron diffraction and an overview of what crystals can be used for, followed by a final closing.



A hands-on session on structure solution.

The social aspects of the school were also not forgotten. On the opening evening of the school there was a well attended mixer to give students the opportunity to meet each other and the tutors and lecturers. On Wednesday afternoon there was an excursion to the wine estates Zorgvliet for wine tasting or Tokara for olive oil tasting and Spice Route, where the participants had a choice of wine, beer, gin, chocolate and charcuterie tastings. This was followed by dinner at the pizza restaurant on Spice Route wine estate. The farewell function on 13 July was a 'spitbraai' - lamb roasted on a spit - accompanied by a variety of local wines.



Enjoying a well-earned break at Zorgvliet wine estate.

Feedback from the participants was positive. General feedback highlighted that many participants really enjoyed the hands-on experience gained at the school, and in fact would have liked more of this. The overwhelming feeling was that a school like the ECS should be a regular event in Africa. In this context it is worth noting that there were a significant number of registrants who were unable to attend the school despite being awarded a partial bursary, because they were unable to source the remaining funding required. This is perhaps an important point to consider when discussing the development of crystallography in Africa; the obstacles faced by researchers range from access to equipment (many participants would have liked to spend more time during the school using a diffractometer) to funding for research (some must buy research chemicals with their own money) to being granted a visa to travel within Africa. These points, among others, were highlighted at the [summit in Bloemfontein during IYCr2014](#). Crystallographers in Africa will need to work together to address these problems. Meetings such as the upcoming [Second Pan African Conference on Crystallography](#), as well as the efforts to promote an African Crystallographic Association, are exciting steps towards meeting these challenges.

Specific feedback from participants was also overwhelmingly positive, as Augustin Nana Nkwento of University of Yaounde, Cameroon, says: "My participation in the ECS5 at the University of Stellenbosch in South Africa was very beneficial for me". In particular, he found the opportunity to learn crystallography

from eminent professors and analyse some crystals very valuable for his PhD study. He also enjoyed the chance to meet and exchange thoughts and ideas with new people from around the world. The ECS5 in Stellenbosch "was not just a school"; Augustin notes that he had a good time discovering the beautiful town of Stellenbosch and visiting the local wine estates. In short, "It was unforgettable". An enthusiastic local participant, Lisa van Wyk of Stellenbosch University, added "The ECS school was unprecedented in the manner that it brought together a variety of skills and knowledge in a setting in Sub-Saharan Africa. In addition, whenever scientists of different fields of specialisation meet there exists great potential for the sharing of unique expertise. Furthermore, it demonstrated that the South African community is in many ways on par with the international community, and we should seek collaborations amongst ourselves as well as abroad."

It is clear that ECS5 was a great learning experience for the participants, and also provided many valuable opportunities to interact with fellow researchers. The (tireless) organising committee are already discussing the organisation of future crystallography schools in Africa – keep an eye out for the first PACS (Pan-African Crystallography School) in the near future!



ECS5 was funded by a number of organisations, to whom we would like to express our sincere gratitude: the ECA, the IUCr, the Italian Crystallographic Association, the Cambridge Crystallographic Data Centre, the South African Chemical Institute, MiTeGen, Bruker, Malvern Panalytical, *Crystal Growth and Design*, Wirsam Scientific, SASOL, the Royal Society of Chemistry (Dalton Division) and *CrystEngComm*.

Photographs courtesy of Delia Haynes and Isabella Claassens.

MEETING REPORT

French Crystallography Association - 2018 meeting report and upcoming events

Philippe GuionneauDominique Luneau



The biennial conference of the French Crystallography Association (AFC), [AFC2018](#), was held in Lyon, the third most populated city in France, which bears witness to 2000 years of history. A total of 227 participants enjoyed high-level science and lively discussions from 10 to 13 July 2018. The scientific program consisted of 3 plenary lectures and 19 sessions, of which 4 were common to all participants and 15 were held in parallel, as well as numerous other events. Excellent pedagogical plenary lectures gave overall views on diverse topics including magnetic chirality (Virginie Simonet, Grenoble), multidrug ABC transporters (Kaspar Locher, Zurich) and applications of mixed metal compounds (Katharina Fromm, Fribourg). The 15 parallel sessions successfully covered most of the present concerns of crystallography in chemistry, physics and biology, as well as making deep incursions into mineralogy and pharmacy. More than 63 talks were delivered within these parallel sessions, leading to a high attendance and numerous questions and comments. During the initial building of the program, particular attention was paid to the involvement of women in order to support the "women in crystallography" movement. Among the plenary sessions, two were dedicated to large-scale facilities. Representatives from SOLEIL and ESRF came to discuss the technical and scientific future of the synchrotrons and their beamlines. Intense and direct discussions were appreciated by all and laid the foundation stone for a deeper reflection that AFC will closely follow. Another common session was dedicated to crystal growth, marking the very strong involvement of the French crystal growth community in the AFC. The last common session, dedicated to teaching, opened up - quite surprisingly - some optimistic prospects on the return of crystallography to

the teaching of students in many places. In addition, the AFC invited the French Neutron Society (SFN) to a special session in order to reinforce the links - already strong however - between these two communities.

Poster sessions were heavily attended and resulted in appreciated poster prizes. AFC also delivers every even year PhD prizes covering biology, chemistry and physics topics. The three winners for 2018 - Clément Charenton (Paris-Saclay), Cassandre Kouvatas (Rennes-Lille-Caen) and Virginie Thery (Limoges) - gave lectures illustrating the dynamism of the young French crystallographers. Other sessions completed this very dense program. Among them, the now recurrent "Meet the industry" session, which involved many industrial workers and notably confirmed that, yes, it is possible to make a career in industry after an initial training in crystallography. Two popular science lectures were also offered to all participants and beyond. Chantal Abergel (Marseille) presented the fascinating and curious universe of giant viruses, while Marie-Hélène Reynaud (Annonay) narrated the difficult but productive life of one of the most famous crystallographers, Auguste Bravais, born near Lyon in 1811. In parallel, the popular travelling science exhibition "Bling Bling! l'art de scruter la matière" created by colleagues from Nancy was on display throughout the meeting. Exchanges with AFC sponsors and exhibitors were possible, notably during the coffee breaks and the Banquet Dinner, which took participants on a cruise to the confluence of the Saone and Rhône rivers, which irrigate Lyon.



A view of the popular science exhibition.

Last but not least, the general assembly of the AFC took place during the meeting and was an opportunity to present an overview of the actions carried out by the AFC over the past two years and to highlight several novelties. Among them, the AFC has created a national prize for confirmed crystallographers that will be awarded every even year, starting in 2020. This prize will be called the AFC "André Guinier" Prize, named after the famous French crystallographer, one of the founders of the AFC and Past President of the IUCr.

The next general conference of the AFC will be organized in Grenoble in July 2020 (Organizing Committee Chairs: Matias Velazquez and Claire Colin). Before then, French crystallographers will meet in

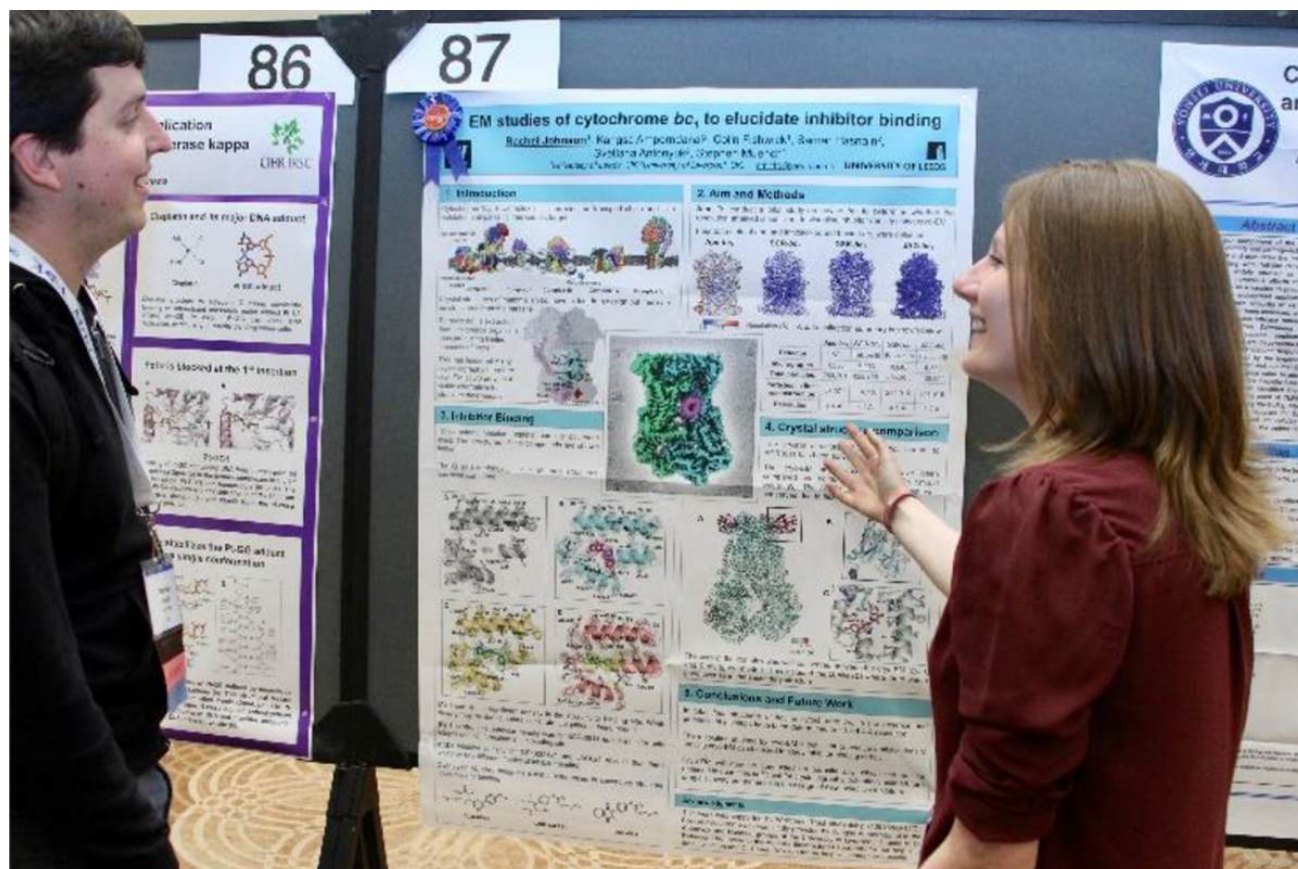
Toulouse for the Integrated Structural Biology meeting jointly organized by AFC and the French Biophysics Society (SFB) from 7 to 10 October 2019, and for the well-established "[Rayons X et Matière](#)" [meeting](#) organized in Nancy from 19 to 22 November 2019.

More details on the above can be found on the AFC web site [here](#).

MEETING REPORT (IUCR SUPPORTED)

68th Annual Meeting of the American Crystallographic Association: the impact of IUCr support

Gerald F. Audette Tiffany L. Kinnibrugh



IUCr poster awardee Rachel Johnson (right) standing by her poster titled “EM studies of cytochrome bc_1 to elucidate inhibitor binding”.

The Annual Meeting of the American Crystallographic Association (ACA) was held from 20 to 24 July 2018 in Toronto, ON, Canada. The IUCr generously provided support in the amount of USD9000 to support travel to the meeting for our young scientists. In general, the meeting on a whole had 663 attendees from 26 countries. Of the 663 attendees, 560 were from the USA and Canada, while 113 (16%) were international. In terms of gender representation, 29% of attendees (193) were female.

In regards to the travel awards, in total there were 62 applicants for travel funds from the ACA and IUCr. All applications went through the ACA registration portal, and awardees were selected by the ACA Education Committee. Of the 62 applications received, 30 individuals were awarded travel funds from ACA/IUCr funds. Of these 30 awards, 12 were awarded from IUCr funds. Demographically, of the 12 IUCr travel awardees, 5 were female (42%) and 3 were international students (not USA/Canada). The average award for a domestic (Canada/USA) student was USD599, and international students received USD1200.

All IUCr and ACA travel awardees were requested to provide a statement regarding their attendance to the meeting and indication of the benefit of the awards to their attendance at the meeting. We have compiled the responses for the IUCr awardees, which are found below.

Rachel Johnson (University of Leeds, UK) received the IUCr poster award for the poster titled “EM studies of cytochrome bc_1 to elucidate inhibitor binding”. In addition, she also received an IUCr travel award to help fund her trip.

We wish to again thank the IUCr for their generous support of funds to facilitate the travel of students to the 2018 ACA meeting. The support of the IUCr in assisting young scientists in attending the meeting is truly appreciated by the awardees, and the regular members who are thus provided the opportunity to interact with these up-and-coming scientists.

Awardee Statements

Mitchell DiPasquale (University of Windsor, ON, Canada)

As an early-career graduate student, the ACA annual meeting in Toronto was my first true conference experience. Being a soft matter researcher, the meeting offered an unparalleled experience to connect with not only leading researchers in my field, but also others in the crystallographic community. Moreover, the event created opportunities to develop myself as a researcher, as well as to interact with a diverse range of industries to discuss the application of current crystallographic technologies to the realm of soft matter. I was able to fully enjoy my first conference experience, partly owing to the travel funding from the ACA facilitating logistics. My experiences at the 2018 ACA Annual Meeting have undoubtedly pioneered my growth as a researcher, and I look forward to the experiences future meetings will bring.



Speakers in Session 3.2.4: Scattering Strategies in Biomembrane Research. (Left to right) John Katsaras, Michael H.-L. Nguyen (IUCr travel awardee), Haden L. Scott, Frederick A. Heberle, Maikel C. Rheinstadter, Mitchell DiPasquale (IUCr travel awardee), Michihiro Nagao, Brett W. Rieckard and Drew Marquardt.

Rachel Johnson (University of Leeds, UK)

I am very grateful to the ACA/IUCr for providing me with the support to travel to the Annual Meeting in Toronto. At the meeting, the quality and diversity of the talks particularly impressed me. The workshop/talks on cryo-EM and the transactions symposium on structure-based drug discovery allowed me to build upon my current knowledge whilst providing me with new ideas to apply to my current PhD research project. Moreover, the diverse range of talks enabled me to engage in research with which I was unfamiliar. For instance, the session on crystallization on the International Space Station was a particular highlight. At the conference, I was also able to present my work in the form of a three-minute thesis talk and a poster presentation where I enjoyed discussing my work with colleagues from around the world. Presenting my work also enabled me to win my first poster prize, so I would like to once again thank the ACA/IUCr for their support.

Rebecca McAuliffe (University of Illinois, Urbana-Champaign, IL, USA)

Thank you again for the support to attend the 68th Annual Meeting of the American Crystallographic Association. At this conference, I was able to present my research and network with several new research and industry groups. The Career Development session and the workshops were especially helpful. I was able to discuss different career opportunities that I had not previously explored, and I was able to learn new about software that will allow me to analyze my data more effectively. I am very grateful for this opportunity and hope to attend this conference again in the future.

Michael Hai-Luu Nguyen (University of Windsor, ON, Canada)

My time at the ACA conference held in Toronto this year was full of exuberant and thought-provoking moments. With the help from the ACA/IUCr travel award, accommodation planning was extremely straightforward and stress-free, allowing me to spend more of my time on my presentation and deciding which workshops I could attend to get the most benefit from this trip. As this was my first major presentation in front of premier experts, I was able to present not only my research but myself, as a researcher, to my colleagues, displaying my skills and potential as a future collaborator and contributor to the field. Moreover, the mixer and poster sessions were a great way for me to open my mind up to new research possibilities, as well as career opportunities (all the while making friends and forging connections is a bonus too!). For all these reasons and many more, I thank the ACA as well as those that made this event and award possible. Without it, I would not be as confident in myself as I am now.



IUCr travel awardee Michael Nguyen presenting his talk "Proteolipid Interactions: A Flip-Flop Perspective".

Joseph Caleb Chappell (Miami University, Oxford, OH, USA)

Attending and presenting at the ACA conference this year was an incredible opportunity for me and provided significant insight into my own research. Being able to interact with so many top notch crystallographers at once is such an exciting and stimulating experience, and one I won't soon forget. I was also able to reconnect with friends I made at the 2017 ACA summer school, and of course meet some new ones! One aspect I particularly enjoy about the ACA meeting is the tightknit community of scientists the meeting generates, and for that reason and many more I will certainly be attending ACA meetings for the foreseeable future. Thank you to the ACA/IUCr for the funding that made it possible for me to attend this world class meeting.

Matthias Uthoff (University of Cologne, Germany)

Attending this meeting of the ACA was great and very inspiring. I have never presented my work at such a big and international conference before and I was able to start some interesting talks at my poster. During the meeting, I learned a lot about methods and facts related but also totally unrelated to my current research topic and work. It gave me an interesting overview of the field and will certainly aid me in finding a position after finishing my PhD. In addition, I was able to meet new people but also some I already knew from other meetings. Getting together (again) and exchanging our experiences was great. Thank you very much for this opportunity and the organization of this fantastic meeting. I could not have participated without your travel grant.

Jocelyn Newton (Brown University, Providence, RI, USA)

I am immensely thankful for receiving an IUCr travel grant to attend my first ACA meeting in Toronto. Through both the cryo-EM workshop and various sessions, I had the opportunity to learn about the emerging applications and challenges in X-ray crystallography and cryo-EM. Speakers in the Structural Biology of Pathogens and the Structural Biology of Inherited Metabolic Disorders sessions highlighted the importance of integrating various techniques in structural biology to understand the molecular mechanisms of disease. Throughout the conference, it was fascinating to learn how scientists are

studying large macromolecular assemblies, such as the spliceosome and membrane protein networks, that were not previously amenable to structural studies. As I am concluding my PhD thesis project, I appreciated having the opportunity to talk with prominent scientists during the poster sessions and networking events to gain insight into both my current research and future career paths. I would like to reiterate my thanks to ACA and IUCr for making this experience possible.

Jahaun Azadmanesh (University of Nebraska Medical Center, Omaha, NE, USA)

I would like to express my sincerest and deepest gratitude for the funding to attend the 2018 ACA conference in Toronto as a PhD student. Several experiences come to mind that I believe greatly contributed to my knowledge base as a crystallographer. First, I attended a workshop that taught attendees how to utilize programs for molecular modeling, which I believe is indeed a skill needed to be developed to express one's work to the scientific community. Second, I had the opportunity to meet and converse with senior scientists in my field and received both valuable and encouraging advice for my area of study: neutron macromolecular crystallography. Third, I have instigated the use of new methods for my scientific work that I learned through the speakers at this conference. Through my experience as a student attending ACA conferences, I truly believe attending these meetings is a substantial opportunity to develop oneself as a scientist. Any student who attends will receive great benefits from the experience.

MEETING REPORT

Second Southeast Asian Conference on Crystal Engineering

Ally Yeo Ing Chien Edward Tiekin



The [Second Southeast Asian Conference on Crystal Engineering \(SEACCE-2\)](#) was held in August 2018 at Sunway University in Malaysia, being hosted by the [Research Centre for Crystalline Materials](#).

The Conference ran for three days and was followed immediately by a two-day workshop on X-ray diffraction/Hirshfeld surface analysis. Inspiring presentations by Gautam Desiraju, Chen Xiao Ming and JJ Vittal kicked off each day with complimentary presentations in oral (29), poster (24) and, highly successful, flash presentation (15) forms drawn from over 100 delegates coming from Thailand, India, the People's Republic of China, Singapore, Indonesia, Pakistan, Bangladesh and hosts Malaysia. The very full five days were generously supported by two Platinum Sponsors - Rigaku Corporation and Crest Nanosolutions Sdn Bhd. We also acknowledge wonderful support for poster and flash presentation prizes from the IUCr, *Crystals*, *CrystEngComm* and Crest Nanosolutions Sdn Bhd.



The Local Organising Committee.

AWARDS AND PRIZES

Gautam Desiraju awarded ISA Medal for Science 2018



The Academic Board of the Institute of Advanced Studies (ISA) of the University of Bologna, Italy, has awarded the ISA Medal for Science 2018 to Gautam R. Desiraju (IIS, Bangalore, India). The ISA Medal for Science is the highest honour awarded by the Institute to scholars who are acknowledged worldwide for their scientific stature and the broad impact of their research.

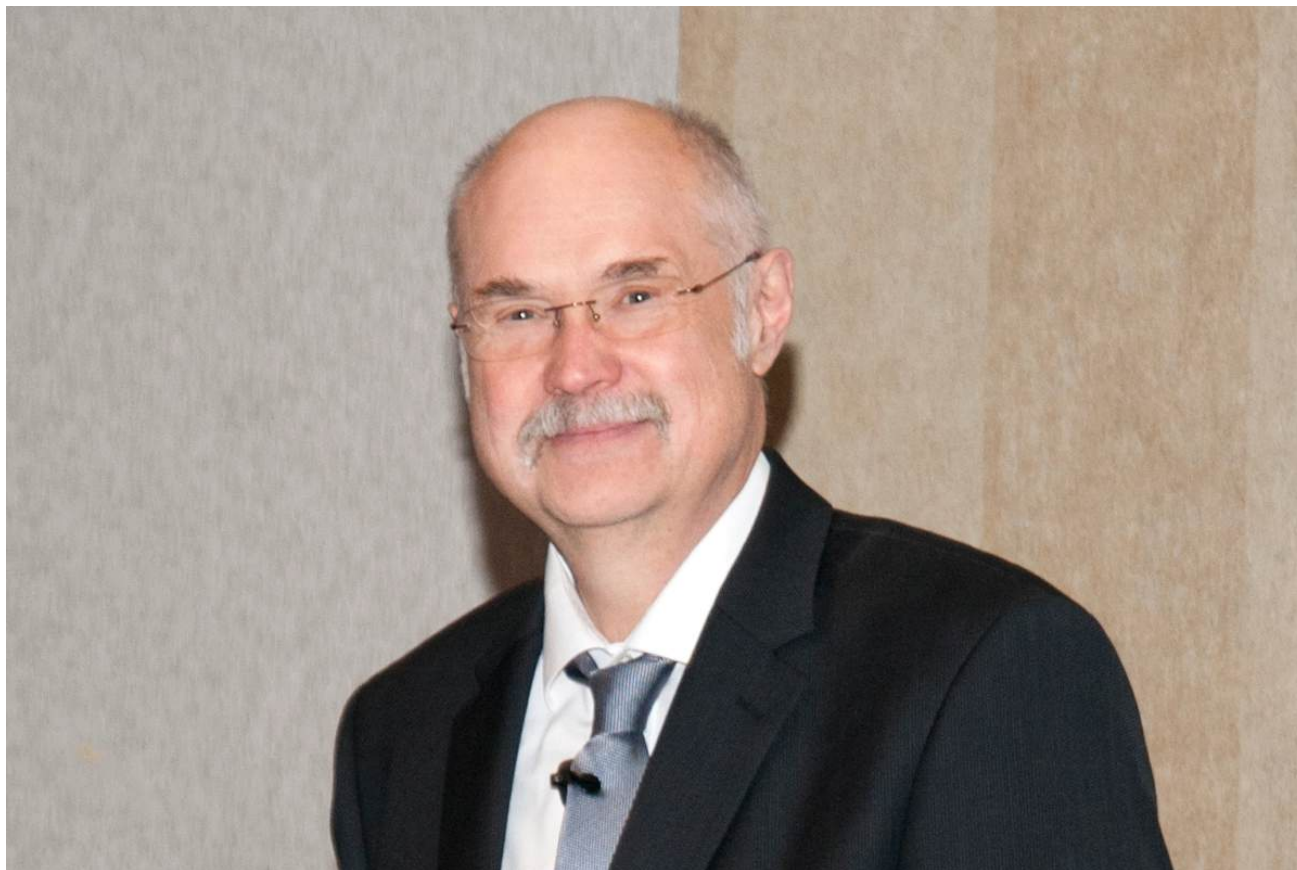
The award ceremony took place on 12 October 2018 in the VIII centenario lecture hall. After receiving the ISA Medal from the Magnifico Rettore, Professor Desiraju delivered the *Lectio Magistralis* "Science and society. What do they owe each other?". A full report will appear in a future issue of the *IUCr Newsletter*.

Professor Desiraju served on the IUCr Executive Committee as President from 2011 to 2014 and as Immediate Past President until 2017, and was Chair of the 2017 IUCr Congress in Hyderabad, India. As a structural chemist, he has played a fundamental role in the development and growth of crystal engineering, bringing his expertise to IUCr Journals *Acta Cryst. B* and currently as Main Editor of *IUCrj*.

AWARDS AND PRIZES

Dmitri Svergun is the 2018 Guinier Prize winner

Jill Trehella



The IUCr Guinier Prize, honouring the great scientist and 'father' of small-angle scattering, André Guinier, is awarded every three years in recognition of lifetime achievement, a major breakthrough or an outstanding contribution to the field of small-angle scattering (SAS).

Nominations for the prize are considered jointly by representatives of the Organizing Committee of the triennial International Small Angle Scattering Conference and the IUCr Commission on Small-Angle Scattering, and presented at the Conference. The [2018 SAS Conference](#) was held in Traverse City, MI, USA, where the 2018 Guinier Prize was awarded to Dmitri Svergun (EMBL Hamburg, Germany) for:

- (i) seminal contributions of innovative methods for the interpretation of SAS data generally, and particularly with respect to biomolecular SAS;
- (ii) sustained effort over several decades to establish and support the most comprehensive suite of data analysis tools for biomolecular SAS in the form of the *ATSAS* program package;
- (iii) leadership in instrument development at EMBL Hamburg, from DORIS to PETRA III; and
- (iv) leadership of and service to the field through community-focused projects and education.

In sum, Dmitri's contributions reflect lifetime achievement as well as outstanding individual contributions to the field of SAS that are most worthy of recognition by the awarding of SAS's most prestigious prize.

Dmitri's scholarly work is documented in more than 500 research publications, including two books, the most recent being a must-have comprehensive reference for both experienced and aspiring small-angle scatterers published as the IUCr text *Small Angle X-Ray and Neutron Scattering from Solutions of Biological Macromolecules* (with co-authors Michel Koch, Peter Timmins and Roland May). Dmitri has generously asked that part of his Guinier Prize money go to enable the IUCr to purchase 30 copies of this text to be awarded as prizes to young scientists at competitions organized at events featuring SAS, including the triennial IUCr Congresses and SAS Conferences, or similar events with prizes for young scientists.

In his presentation at the award ceremony, Dmitri honoured his influential mentors and teachers and the many collaborators, students and post docs he has worked with, beginning with his time as a graduate student at Moscow State University and the Institute of Crystallography in Moscow where he subsequently was appointed to a research position in 1980 to pursue his interests in biomolecular SAS. He continued in this theme through his time when he came to Germany in various visiting and guest capacities at GKSS Geesthacht and then at the EMBL unit in Hamburg where he eventually moved full time, becoming a group leader and then a senior scientist. It was at the EMBL that Dmitri was able to fully realize his vision for biomolecular SAS, in the process building an outstanding team of theoretical, computational and experimental researchers, many of whom have continued in the field with distinction, many of whom were heard from at SAS2018.

Dmitri's seminal contributions are broad and impactful. There was the inclusion of perceptual criteria combined with the automated optimization of the regularization parameter to obtain stable $P(r)$ solutions from indirect Fourier transformation of SAS data. This was quickly followed by the publication of a method to rapidly calculate small-angle X-ray scattering profiles from atomic coordinates, which was a major breakthrough in that it provided the missing link between high-resolution structures and low-resolution solution data - and remained without any competitor for ~15 years before new approaches were developed. A series of further developments gave us a general method for restoring the shape of a scattering object from the solution SAS profile, the means to evaluate the uniqueness of the shape determination and a measure of similarity of models, rigid-body modelling for when atomic coordinates for domain and/or subunit structures are available, options for including flexible linkers, and finally modelling intrinsically flexible proteins in terms of conformational ensembles.

These innovations and advances form the core of the ATSAS program package for SAS data manipulation, analysis and modelling that is under continuous development and enhancement and is used extensively in the biomolecular SAS community. Its popularity is no doubt not only due to its versatility but also to the fact that it is well documented, freely available for download for academic users, accessible via an online service, and that users are supported via the online Saxier forum or as needed via collaborative engagement.

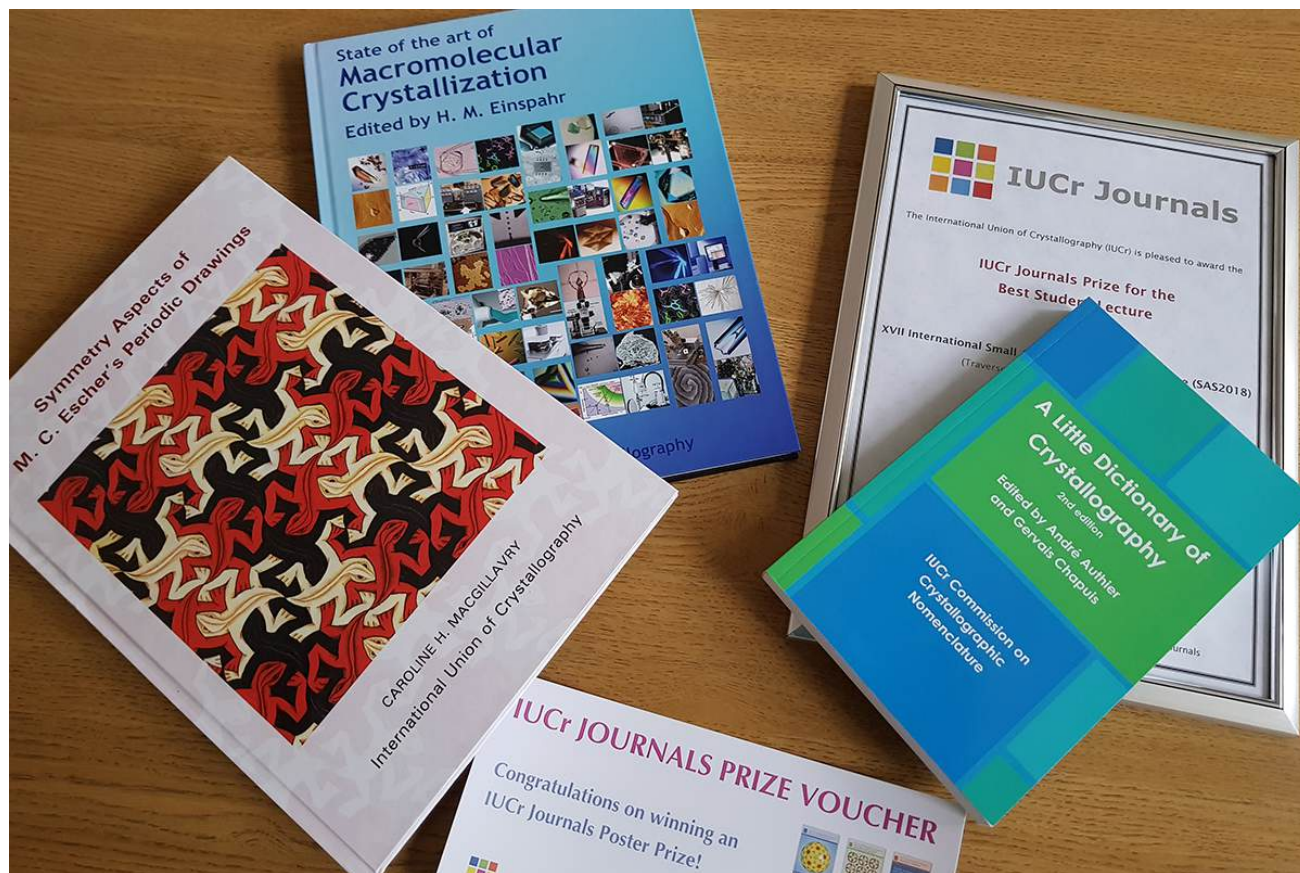
Data analysis tools are of little value without high quality data, and so in addition to this work, Dmitri ensured the continued tradition of innovation at the SAS facilities in Hamburg, first at DORIS and now Petra III, with automation of sample handling, inline sample purification and characterization, and on-the-fly analyses.

Dmitri's impact extends well beyond the boundaries of SAS. Recognizing the value of combining complementary data to advance our molecular understanding of biology, Dmitri's educational outreach soon moved beyond his popular Hamburg-based practical SAS courses to organizing global lecture series for structural biology that combined SAS with complementary biophysical methods. He took them to China, Korea, Brazil, India, Taiwan and Singapore (so far), spreading the power of SAS with good practices to other scientific communities and helping to grow the number of SAS users all over the world. His ongoing collaborative work with the worldwide Protein Data Bank on initiatives to support hybrid methods for solving complex structures provide a crucial foundation for SAS to contribute to this important emerging frontier.

Dmitri is a Co-editor of *J. Appl. Cryst.*

AWARDS AND PRIZES

IUCr Journal prizes



The IUCr would like to congratulate the following winners of IUCr Journals best student presentation/poster prizes. More to follow in the next issue!



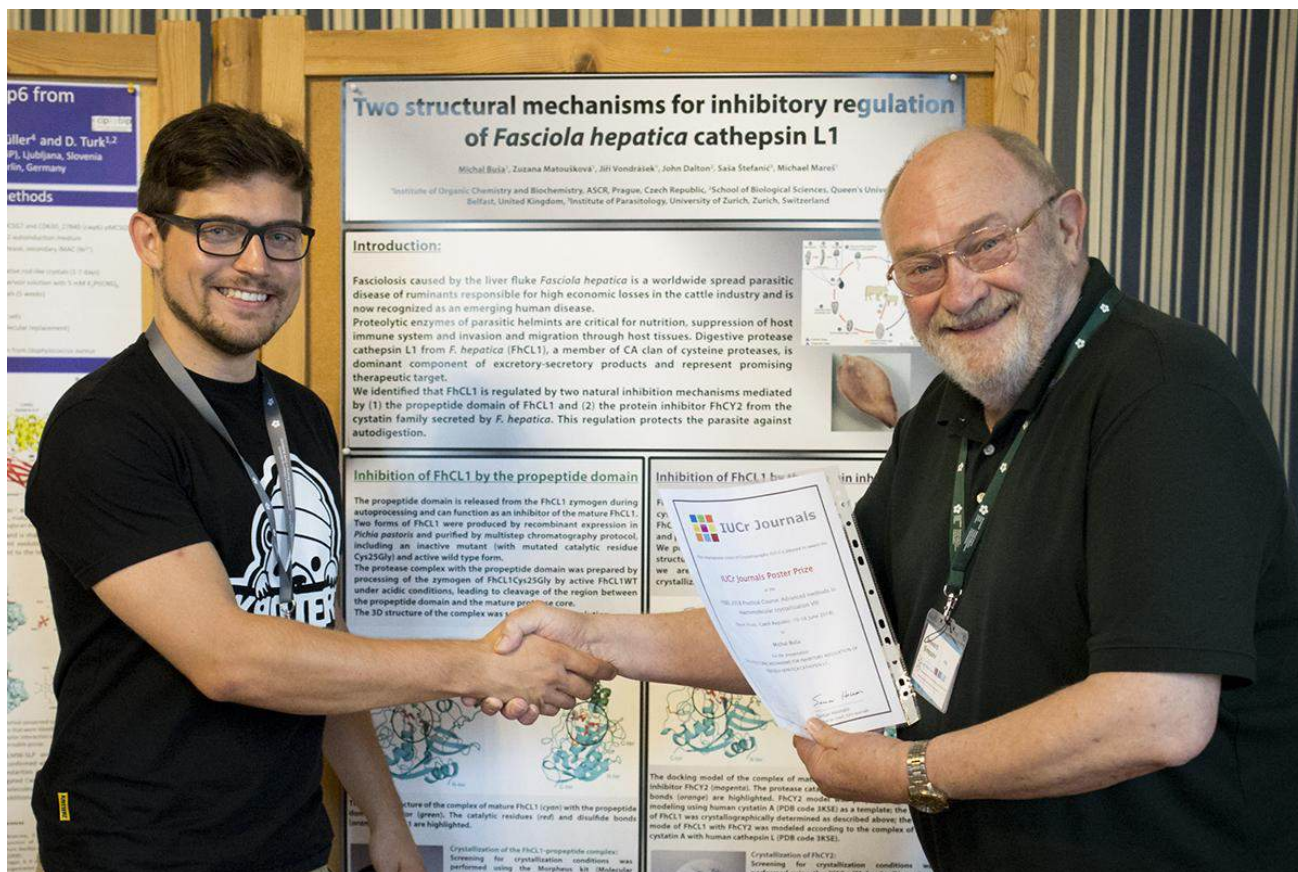
Hans Hendrikse (right) (AMOLF, the Netherlands), poster "Two Worlds Collide: Biomineralization and Functional Materials", 6th International School of Crystallisation (Granada, Spain; 20-25 May 2018). Prize presented by Juan Manuel García-Ruiz, School Director (left), and Giuseppe Falini, Jury Chair.



Francesca Carella (right) (Istec-CNR, Italy), poster "Three-dimensional matrices of enamel like oriented calcium phosphate nanocrystals", 6th International School of Crystallisation (Granada, Spain; 20-25 May 2018). Prize presented by Giuseppe Falini, Jury Chair.



Veronica Iuliano (centre) (University of Salerno, Italy), poster "Solvatochromic properties and solid-state inclusion of a *p*-pyridinium-calix[4]arene", 2nd PoMoS (Vietri sul Mare, Italy; 6-8 June 2018). Prize presented by Susan A. Bourne (left) and Consiglia Tedesco, Conference Chair.



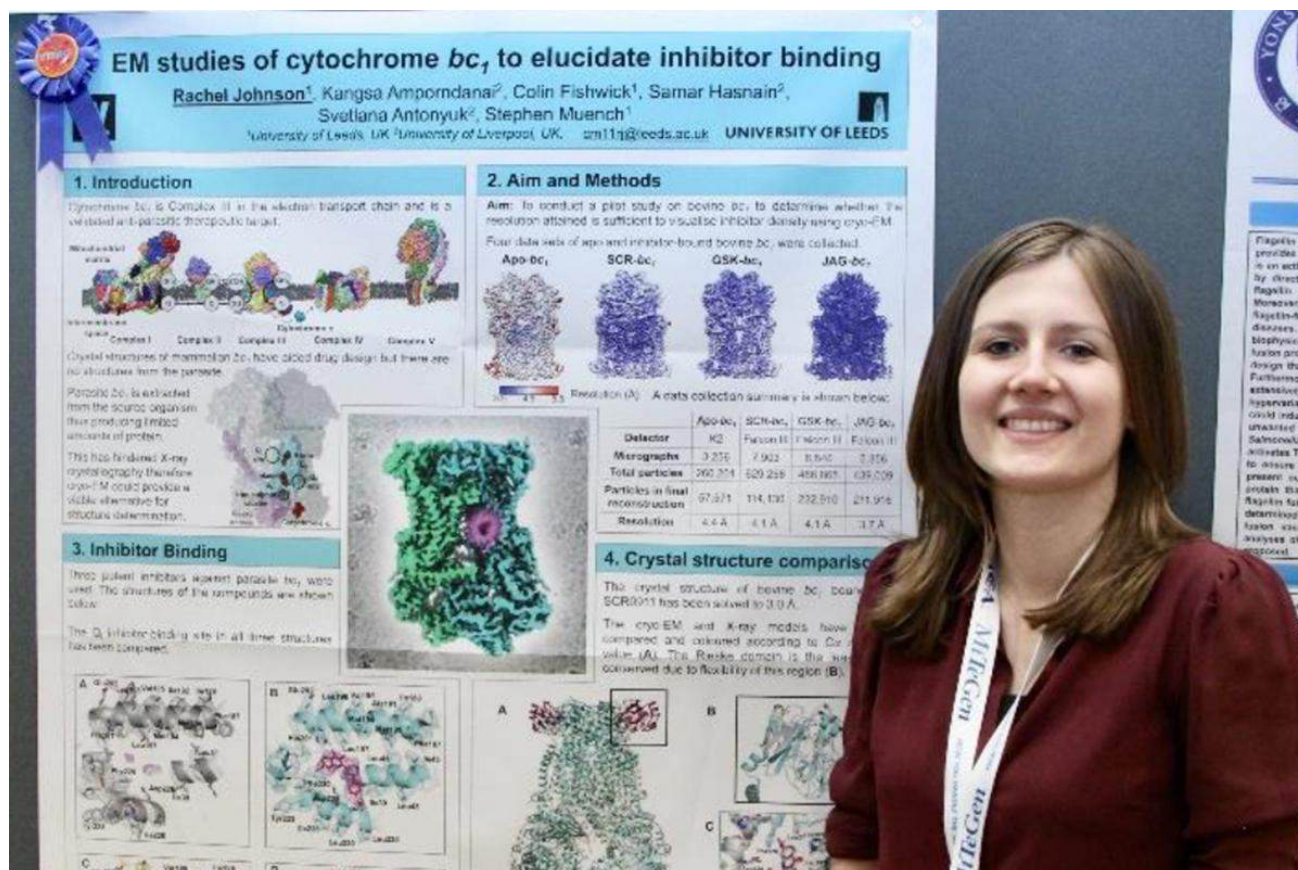
Michal Buša (left) (CAS, Prague, Czech Republic), poster "Two structural mechanisms for inhibitory regulation of *Fasciola hepatica* cathepsin L1", FEBS 2018: Advanced methods in macromolecular crystallization VIII (Nové Hradý, Czech Republic; 10-16 June 2018). Prize presented by former *Acta Cryst. F* Editor Howard Einspahr.



Lidija Kanižaj (right) (Rudjer Bošković Institute, Zagreb, Croatia), lecture "Chloride- and oxalate-bridged heterometallic $[\text{Cu}^{\text{II}}\text{Cr}^{\text{III}}]$ compounds with 2,2':6',2''-terpyridine – the influence of the starting copper(II) salt", CSCM26 (Poreč, Croatia; 13-17 June 2018). Prize presented by Michele Zema, IUCr Executive Outreach Officer.



Ivana Kekez (left) (University of Zagreb, Croatia), lecture "Revealing the structure of the first plant aminoacyl-tRNA synthetase at 2.3 Å", CSCM26 (Poreč, Croatia; 13-17 June 2018). Prize presented by Michele Zema, IUCr Executive Outreach Officer.



Rachel Johnson (University of Leeds, UK), poster "EM studies of cytochrome bc_1 to elucidate inhibitor binding", 68th Annual ACA Meeting (Toronto, Canada; 20-24 July 2018).



Suman Bhattacharya (right) (University of Limerick, Ireland), poster "Temperature-dependent Phase Switching in a 2D Layered MOF", Second Southeast Asia Conference on Crystal Engineering (Sunway University, Malaysia; 6-8 August 2018). Prize presented by Edward Tiekink, Conference Chair and *IUCrData* Editor.

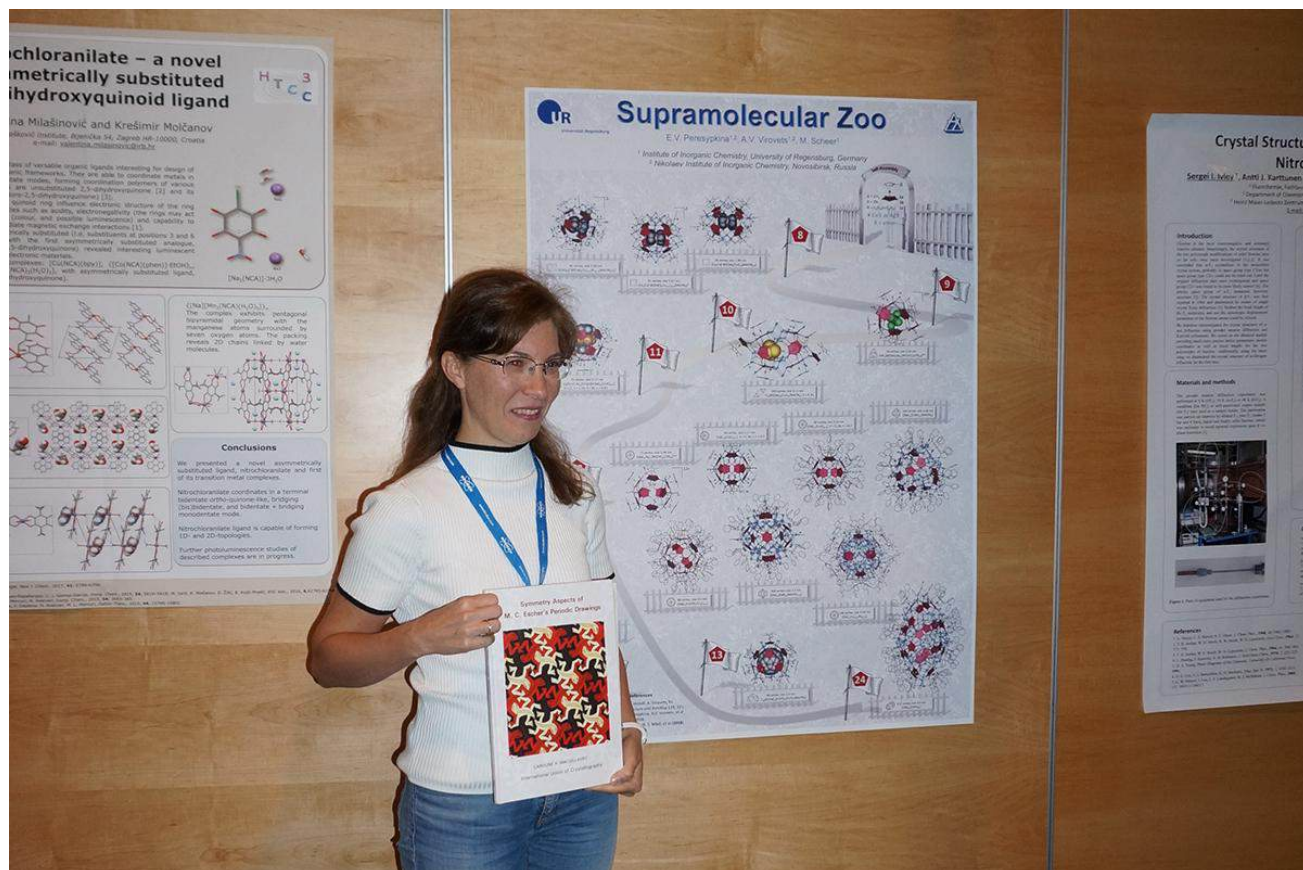


Christian Jenewein (left) (University of Konstanz, Germany), poster "Binary Mesocrystals from Anisotropic Nanoparticles", ECCG6 (Varna, Bulgaria; 16-20 September). Prize presented by Andrea Zappettini, Chair of the IUCr Commission on Crystal Growth and Characterization of Materials.



Saša Petrović (centre) (MDC, Berlin, Germany), talk "Structural basis of ASPL-mediated regulation of p97 methylation by METTL21D", HEC21 (Quedlinburg, Germany; 20-22 September 2018). Prize presented by Milton T. Stubbs (far left), Kristina

Djinovic-Carugo, Chair of the Judging Committee (second from right) and Michael Rossmann (far right), Editor of *International Tables* Volume F.



Eugenia V. Peresypkina (Institute of Inorganic Chemistry, University of Regensburg, Germany), poster “Supramolecular Zoo”, Hot Topics in Contemporary Crystallography 3 (Bol, Croatia; 23-27 September 2018).



Andrew McCluskey (centre) (University of Bath, UK), lecture "*pylj*: An Open-Source Python Library for Teaching the Interaction between Molecular Simulation and Scattering", SAS2018 (Traverse City, MI, USA; 7-12 October 2018). Prize presented by Andrew Allen, Editor-in-Chief of IUCr Journals, and Jill Trehwella, IUCr Commission on Small-Angle Scattering.

OBITUARY

José Lima-de-Faria (1925-2018)

Giovanni Ferraris



On 27 May 2018, the eminent Portuguese crystallographer José Lima-de-Faria passed away in Lisbon, where he was born on 17 June 1925. José was the youngest of four children; his father was a notary and his mother belonged to a family of republican tradition, being herself an activist engaged in a women's republican association.

Initially oriented towards engineering, during the last year of high school he was strongly encouraged by his philosophy teacher to follow the path of scientific research, which better matched his interests. From early on, besides science, he developed profound interests towards diverse subjects of art, philosophy, history and literature, which made him a collector of books, objects (naturalist collection) and ideas. He was known for his sense of humour and storytelling and as a big fan of Charlie Chaplin.

After obtaining a degree in physical and chemical sciences (Faculty of Sciences, University of Lisbon, 1950), José moved to Paris, France, where he worked for about two years in a stimulating scientific environment under the supervision of Louis De Broglie. In the period 1959-1962, he entered as a research student the Department of Crystallography at Cambridge University, UK, where, under the supervision of Peter Gay, he obtained a PhD in crystallography and mineralogy.

José started his professional research career in Lisbon as a member of the Scientific Group of Geology attached to the Faculty of Sciences, and became a researcher of the Junta de Investigações do Ultramar (1956). He was further responsible for the establishment of the Laboratory of Physical-Chemical Techniques Applied to Mineralogy and Petrology and of the Laboratory of Petrological and Paleontological

Studies of the Board for Overseas Research (1956-1959). In 1995 he formally retired, but kept his functions as director of the Centre for Mineralogy and Crystallography and of the Department of Earth Sciences of the Tropical Research Institute (former Junta de Investigações do Ultramar) till 2003.

José actively served the international crystallographic and mineralogical communities as a member of the IUCr Teaching Commission and chairman of its Nomenclature Commission (1984-1990) and a member of the Mineral Classification Commission (1989-1998) of the International Mineralogy Association.

He began his research activity studying low-crystalline metamict minerals by X-ray powder diffraction - not an easy task - obtaining results published in the book *Identification of Metamict Minerals by X-ray Powder Photographs* (Junta de Investigações do Ultramar, Lisbon 1964), which became an important reference work in that field. This research acted as a training to develop new ideas on the crystal chemistry and the structural classification of minerals, a field where José emerged as an original leader. On these subjects he published, partly in collaboration with Maria Ondina Figueiredo, a series of articles in international journals and the following innovative and successful books: *Structural Mineralogy. An Introduction* (Springer Netherlands, Dordrecht 1994) and *Structural Classification of Minerals* (three volumes; Springer Netherlands, Dordrecht 2001, 2002, 2003).

At the same time, José developed a strong interest in the history of crystallography and edited the well known *Historical Atlas of Crystallography* (Springer Netherlands, Dordrecht 1990). In fact, he was firmly convinced that the teaching of science improves with the simultaneous teaching of its history because scientific discoveries are often the result of the accumulation of several advances in relation to a certain problem that, at one point, takes a more definitive form.

José is survived by his wife, Maria Natália, and their children, Margarida and Manuel.

*This article was originally published in [J. Appl. Cryst.](#) (2018), **51**, 1507-1508.*

OBITUARY

Aafje Looijenga-Vos (1928-2018)

Bram Schierbeek



Aafje Vos during the Eighth IUCr Congress in Stony Brook, NY, USA, in 1969.

Aafje Looijenga-Vos, emeritus professor of structural chemistry at the University of Groningen, the Netherlands, died at the age of 90 on 4 November 2018.

Aafje Looijenga-Vos was professor of general chemistry from 1962 to 1967 and professor of structural chemistry from 1967 to 1983 at the University of Groningen. She was one of the founders of crystallography in general and of Dutch crystallography in particular.

Aafje was born in Marum in the north of the Netherlands. After her secondary school, in 1946, she started studying chemistry at the University of Groningen. In her first year she heard a lecture by Professor Eelco Wiebenga about X-ray crystallography and was impressed by the idea that it would be possible to actually see individual atoms lie next to one another. During her studies she met other Dutch crystallographers at the national meetings: Bijvoet from Utrecht, MacGillavry from Amsterdam and de Wolff from Delft as well as other international crystallographers during the first IUCr Congress in 1948. She finished her studies in 1952 and started a PhD in the lab of Professor Wiebenga. For her thesis work she employed Patterson methods to solve the structures of P_4S_{10} and P_4S_7 , compounds that already intrigued her during her organic chemistry practicals. After crystallization of the compound it took her nine months to measure the intensities of about 1000 reflections on film and calculate the necessary three-dimensional Patterson function. The two structures [1] were the basis of Aafje's thesis, which she defended and earned with praise in 1955.

Aafje stayed at Groningen University. During the first two years she worked at UK crystallographic institutes in Glasgow, Leeds, Oxford and Cambridge. In Oxford she worked closely together with Dorothy Hodgkin, who was close to finishing the structure of Vitamin B₁₂ [2]. While mending socks in the garden of Dorothy's house, they discussed crystallographic problems.

In 1962 Aafje became professor of general chemistry and in 1967 professor of structural chemistry at the University of Groningen. In this new role she also worked in American institutes in Buffalo, Washington DC, Oak Ridge, Brookhaven and Pittsburgh. In Buffalo she visited Philip Coppens and together they performed neutron diffraction experiments on cyanuric acid crystals at Brookhaven National Laboratory [3]. In Washington DC she worked on direct methods with Isabella Karle at the Naval Research Lab. There she showed in just over one day how an organic compound looked completely different from what the organic chemists expected [4]. Together with the group in Utrecht and the company Enraf-Nonius in Delft, Aafje stood at the cradle of the development of the CAD-4, the Computer Automated Diffractometer with 4 circles. One of the first of these instruments was installed in her lab in 1969. This made it possible for her co-worker Jan de Boer to measure accurate intensities in an automated way [5]. It also led to the foundation of the centre for participation research [6] in Utrecht in the early 1970s where Ton Spek measured crystals and solved X-ray structures for third parties.

Aafje's crystal chemistry group covered a broad range of topics: cyclophosphazenes [7], electron-density distribution studies using high-resolution data at low temperature [5], relations between structure and electrical and magnetic properties of morpholinium-TCNQ compounds [8], combining force-field calculations with X-ray measurements on compounds that are "sterically hindered", incommensurable structures and biologically active peptides [9].

Next to her research activities she was active in a number of roles: prior to the 10th IUCr Congress in Amsterdam in 1975, Aafje chaired the programme committee of the conference. From 1977 to 1982 she was secretary of the IUCr Commission on International Tables and with her wit and her charm and organisational skills she played a big role in bringing together the views of many crystallographers from Europe and the rest of the world and realising the 1983 edition of *Volume A of International Tables for Crystallography*. In 1980 she became a member of the Royal Dutch Academy of Sciences.

In 1982 she suddenly announced that, at the age of 54, she would marry Hans Looijenga, a widower with eight children, and move to the west of the Netherlands. A career change indeed and quite a surprise for me, having just started a PhD in her lab.

She smoothly blended into her new family as a spouse and stepmother and later as a grandmother, but her new role did not stop her being active in science. She kept on visiting the yearly Dutch crystallographic meetings in Luntenen, and from 1987 to 1990 she was secretary of the Free section of the Royal Dutch Academy of Sciences.

Her memoirs (in Dutch) entitled '*Memories of Crystal Chemistry*' are published in a compilation of memories of 24 Dutch researchers in Chemistry (Delft University Press, 1993) and can be accessed [here](#) as a pdf file. Aafje concludes that, with the increasing speed of data collection and computing, many new areas are being developed by crystallography. "... and yet, what a great charm the old handicraft had!"

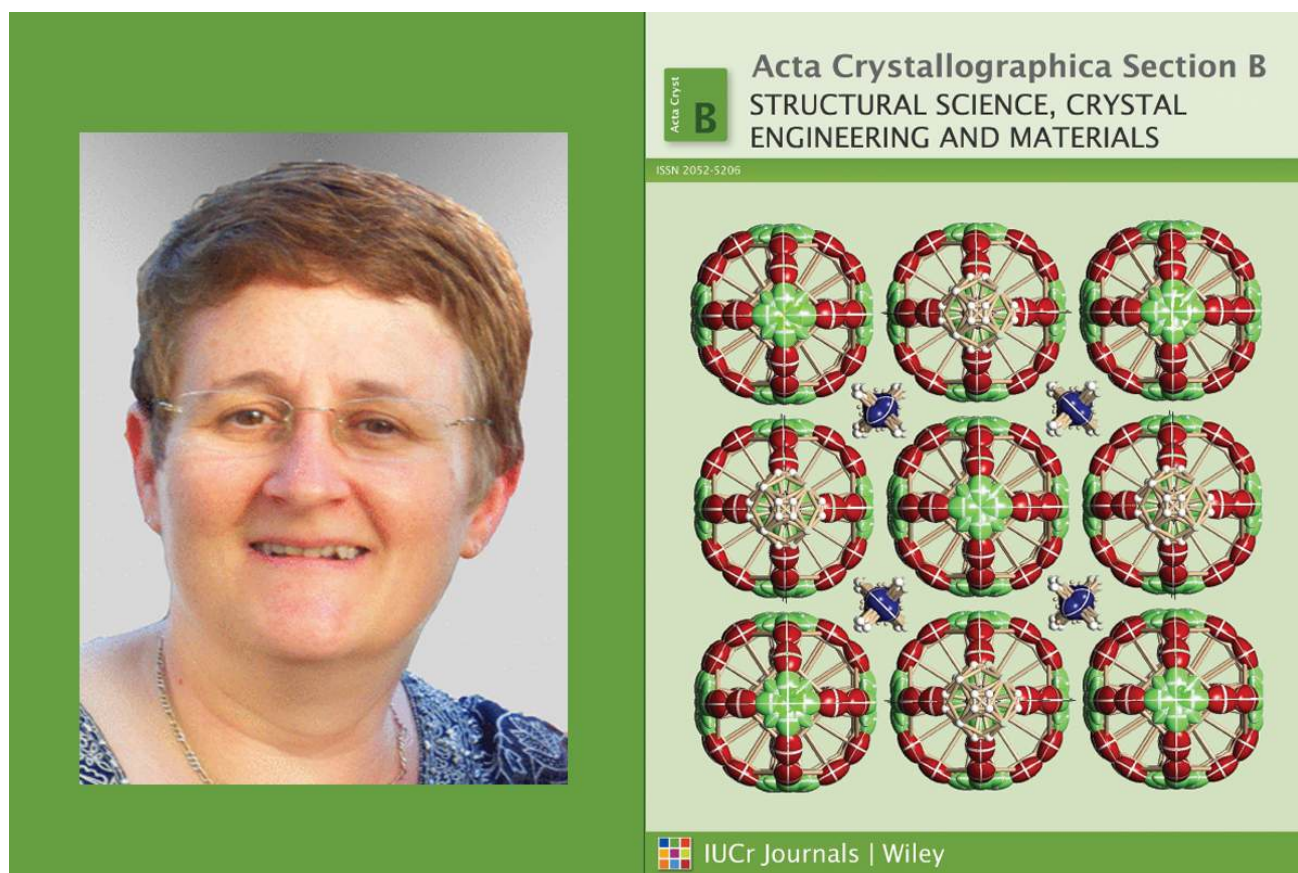
Aafje Looijenga-Vos is survived by 21 grandchildren and 4 great-grandchildren.

References

- [1] A. Vos & E. H. Wiebenga (1955). *Acta Cryst.* **8**, 217-223.
- [2] D. Crowfoot-Hodgkin *et al.* (1955). *Nature* **176**, 325-328.
- [3] P. Coppens & A. Vos. (1971). *Acta Cryst.* **B27**, 146-158.

- [4] J. C. van de Grampel, A. J. Cuperus & A. Vos (1971). *Recl. Trav. Chim. Pays-Bas* **90**, 587-593.
- [5] J. L. de Boer & A. Vos (1979). *Acta Cryst.* **B35**, 1809-1812.
- [6] The National Single Crystal X-ray Facility, Utrecht University.
- [7] A. J. Wagner & A. Vos (1968). *Acta Cryst.* **B24**, 1423-1430.
- [8] R. J. J. Visser, J. L. de Boer & A. Vos (1990). *Acta Cryst.* **C46**, 869-871.
- [9] G. Admiraal & A. Vos (1984). *Chem. Biol. & Drug Design* **23**, 151-157.

OBITUARY

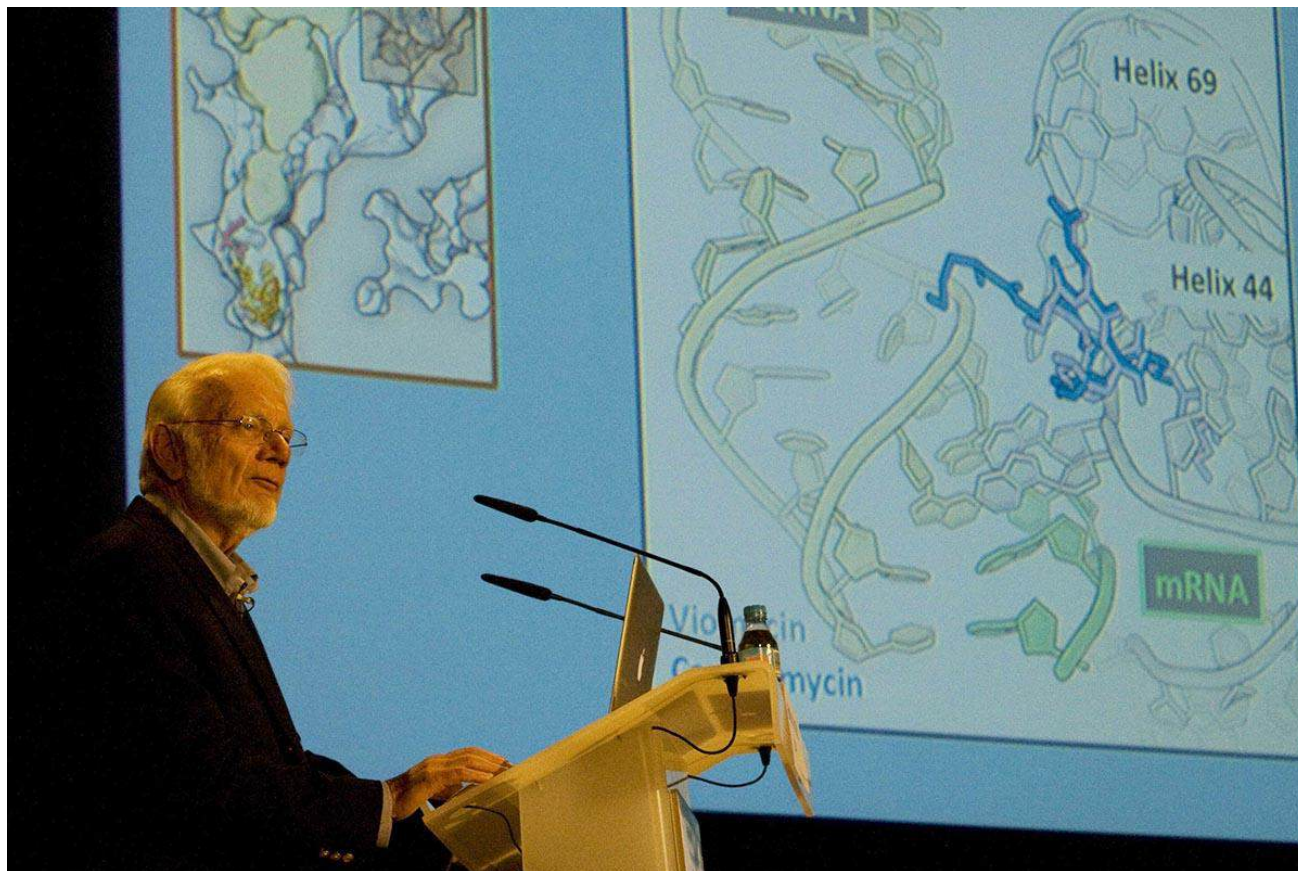
Jill Bradshaw (1968-2018)

We are sorry to report the passing of Jill Bradshaw, following a long illness. Jill was a key member of staff in the IUCr Editorial Office in Chester, where she was the Managing Editor of *Acta Cryst. B*. Jill joined us in the summer of 1993, following a spell as a production editor at Pergamon Press, where she worked after graduating from the University of Sheffield. Jill mainly acted as an editor on *Acta B*, and authors of this journal in particular will remember her for the efficient way that she handled their papers and the kind and diplomatic way in which she handled correspondence and queries.

In the summer this year, we celebrated Jill's 25th anniversary with the IUCr. Jill was determined to attend and, despite being unwell, was able to be cheerful and positive during a long afternoon of celebrations. All the staff in Chester will miss Jill - we have lost a highly valued colleague and friend.

OBITUARY

Thomas A. Steitz (1940-2018)

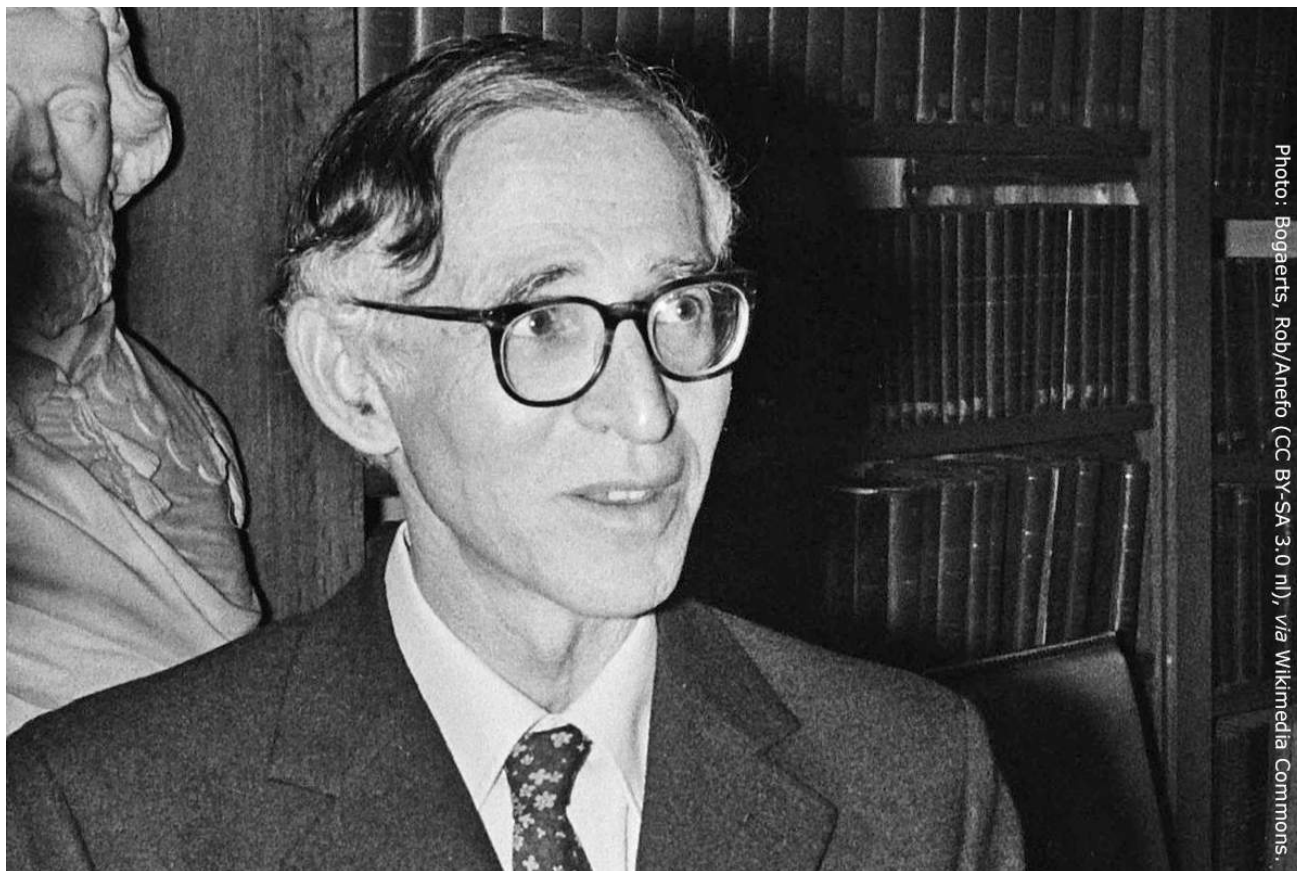


Thomas Steitz, Sterling Professor of Molecular Biophysics and Biochemistry at Yale University, USA, has died at the age of 78. Dr Steitz shared the [2009 Nobel Prize for Chemistry](#) with Venkatraman Ramakrishnan and Ada E. Yonath "*for studies of the structure and function of the ribosome*".

He can be seen above giving his Plenary Lecture "From the Structure and Function of the Ribosome to New Antibiotics" at the IUCr Congress in Madrid, Spain, in 2011. Read the NY Times obituary [here](#) and that in YaleNews [here](#).

OBITUARY

Aaron Klug (1926-2018)



Sir Aaron Klug, a Lithuanian-born, South African-educated British chemist and biophysicist, died on 20 November 2018. He was the sole winner of the [1982 Nobel Prize in Chemistry](#) “for his development of crystallographic electron microscopy and his structural elucidation of biologically important nucleic acid-protein complexes”.

A full obituary will appear in the *IUCr Newsletter* in due course.

OBITUARY

Håkon Hope (1930-2018)



Håkon Hope, member of the IUCr Commission for Crystallographic Apparatus from 1978 to 1984 and Co-editor of *Acta Cryst. B* and *C* from 1984 to 1993, died peacefully at home in Davis, CA, USA, on 22 November 2018. Born in Førde, Norway, he joined the faculty of the Department of Chemistry at UC Davis in 1965, retiring as professor emeritus in 1993.

A full obituary will appear in the *IUCr Newsletter* in due course. Please see that in the *Davis Enterprise* [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