INTERNATIONAL UNION OF CRYSTALLOGRAPHY

IUCr Newsletter

Volume 27 · Number 2 · 2019

Collected archival edition with articles grouped by their original editorial categories, complete text, and available illustrations.

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LETTER FROM THE PRESIDENT

Taxing questions

Sven Lidin



The IPC hard at work.

IUCr2020

The next Congress and General Assembly of the IUCr in Prague is taking shape. Congresses are important because science is a social undertaking: we need to meet, discuss and interact face-to-face to make new contacts, get new ideas and forge new friendships. We are a community with very wide interests and our science impacts many areas in the physical, chemical and biological sciences. It is natural that many of the meetings we attend are not primarily crystallographic but deal with questions where crystallography is but one of the pieces of the puzzle. It is important for the cohesion of crystallography that we also meet among crystallographers to rethink and reinvent our own area of expertise.



Congress Chair Radomír Kužel during a brief rest from the decision making during the IPC meeting in Prague.

The programme for the Congress was discussed intensely and sometimes heatedly during the International Programme Committee (IPC) meeting, which took place from 14 to 17 May 2019. It is an excellent sign of health that we all feel strongly about our science. The multifaceted nature of crystallography makes the difficult choices made by the IPC an *embarras de richesses*. There is no problem in finding topics to include in an exciting programme, the difficulty lies in all the fascinating possibilities for which we find no room this time around. The programme will appear on the website as soon as the invited speakers have accepted. We can hope for a very exciting Congress with excellent science in the city of Prague in 2020.

Tax-exempt status

The IUCr was accepted into the International Council for Science (now the International Science Council) as a scientific union in 1947 and the first General Assembly was held in 1948. From 1969, the Union was legally domiciled in Geneva, Switzerland, as stated in the Statutes and By-laws: *2.3. The legal domicile of the Union is in Geneva, Switzerland*.

This is an interesting arrangement as the working address of the secretariat (the Executive Secretary) and all the permanent staff working for the Union and the Union's journals is in Chester, Great Britain, but it reflects an arrangement that has worked very well over the years and it has allowed the Union to maintain a tax-exempt status that has been

financially beneficial to our operations without the need for a General Assembly to be held annually, as would be the case for many other domiciles, including the UK.

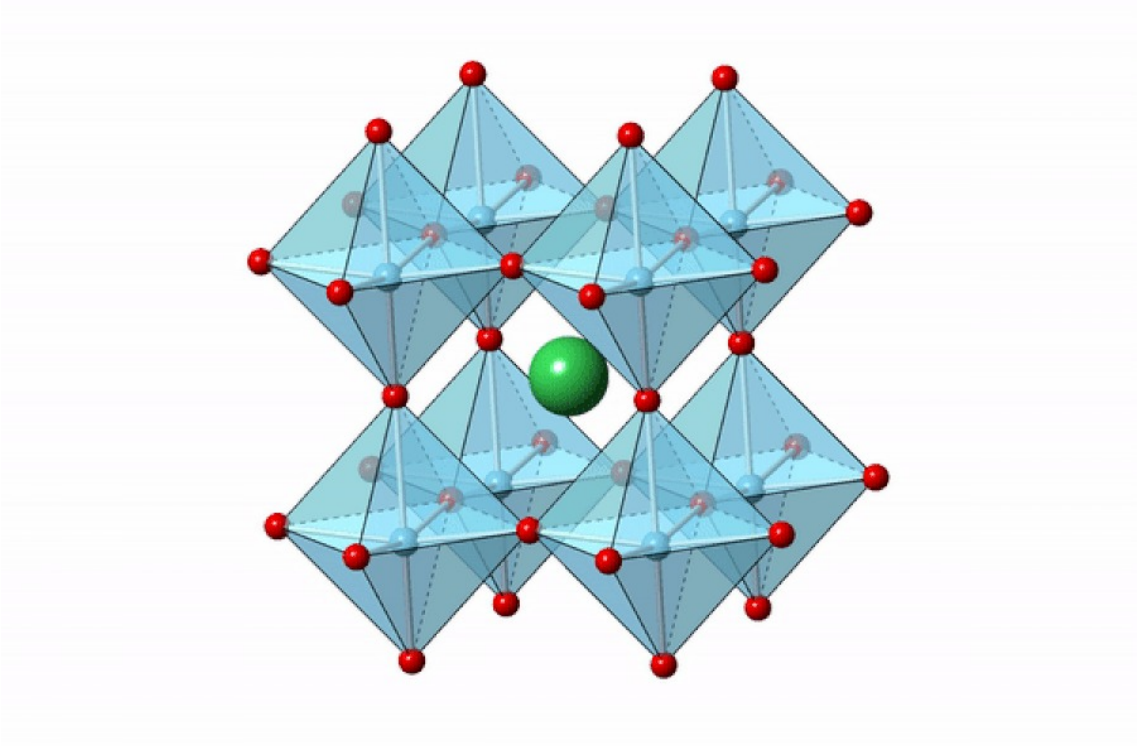
This status has now been questioned by the Swiss tax authorities and their concern is whether the turnover of the commercial branch of the Union is disproportionally larger than the turnover of our charitable branch. The Executive Secretary has therefore started collecting statements from members of our community asking them to estimate the number of unpaid hours they devote to the IUCr each year. We hope that the accumulated number will convince the Swiss authorities that we are indeed a charitable organisation rather than a commercial enterprise. Although there is no guarantee of success, we hope this exercise will help us to profit from a maintained tax-exempt status.

Original article: https://www.iucr.org/news/newsletter/etc/articles?issue=142706&result_138339_result_page=1

EDITORIAL

Crystal clear

Mike Glazer



Massimo strikes again! This time Massimo Nespolo tackles the thorny problem of how to convince fellow scientists that they need to understand the difference between the basic crystallographic concepts of “lattice” and “structure”. Both he and I have for some time been conducting an active campaign to write to editors of journals about this problem, to get them to insist on the correct terminology wherever possible. Lest you should think this is mere pedantry, I have a story that I have repeated many times and do so here too. I think it is worth repeating. Many years ago when I was working at the Cavendish Laboratory in Cambridge, I was approached by a PhD student working on computation of the electronic band structures of certain so-called Laves phases. He had been struggling with this for nearly a year and could not get satisfactory results from the computer program that he was using. Now this was a time well before the era of personal computers, when all computing was *via* mainframe machines, which were expensive to run. Turnaround could be around one week. Anyway, I sat down with him to look at the input requirements for the software and I realised that he was confused about the difference between the number of lattice points in a unit cell and the number of atoms. Once I explained to him the difference, he was then able to get the program to provide sensible answers. He had wasted nearly a year of expensive computer time on this problem fundamentally because of this misunderstanding. As Massimo explains, the origin of this mistaken thinking lies in the way that textbooks tend to describe only very simple crystal structures where there appear to be just one atom per lattice point. So here is a

call to all crystallographers: whenever you spot this mistake in the literature, draw attention to the journal editor and let's see if we can eventually stamp out these errors!

Another article in this issue is once again from Juan Manuel Garcia-Ruiz (his first article on quartz crystals and early hominids was published last year in the *Newsletter*. Quartz again appears here in his article on Indiana Jones and the Crystal Skull, which makes entertaining reading. Several years ago, I was approached by a media company who were planning to make a film debunking the crystal skulls myth. I found a company in Germany who were manufacturing the skulls that were claimed to be even better than the mysterious skulls. The crystal skulls story is another of those endless cases of crystals and pseudoscience. Just type the word "crystals" into Google and see the first sites that come up. I recall several years ago how someone telephoned me to ask about crystals and when I mentioned that crystals are the "deadest" things in the universe he became very upset and even threatened me. Both of these articles illustrate how poorly understood crystallography is in the public mind.

I have also included my own article entitled Bragg's balls using items taken from my own small collection of crystallographic memorabilia. W. L. Bragg was very capable at making things with his own hands and loved to construct models to illustrate various crystallographic concepts simply. He made several models using ping-pong balls cemented together, for instance to illustrate the formation and propagation of dislocations in metals. He also demonstrated in one of his lectures at the Royal Institution of Great Britain how a simple crystal could grow to form a recognisable morphology, simply by using glass marbles. Many years later I built my own version, described here, and have found it a great way to show school students and the public about crystal growth and emphasise the beauty of crystallography. You may like to try this out for yourself.

Also, at a recent crystallography conference I heard an entertaining and fascinating talk by a young man from Malta (James-N Grima-Cornish) on the crystallography of auxetics. What's that I hear you say? Well you can read about that here.

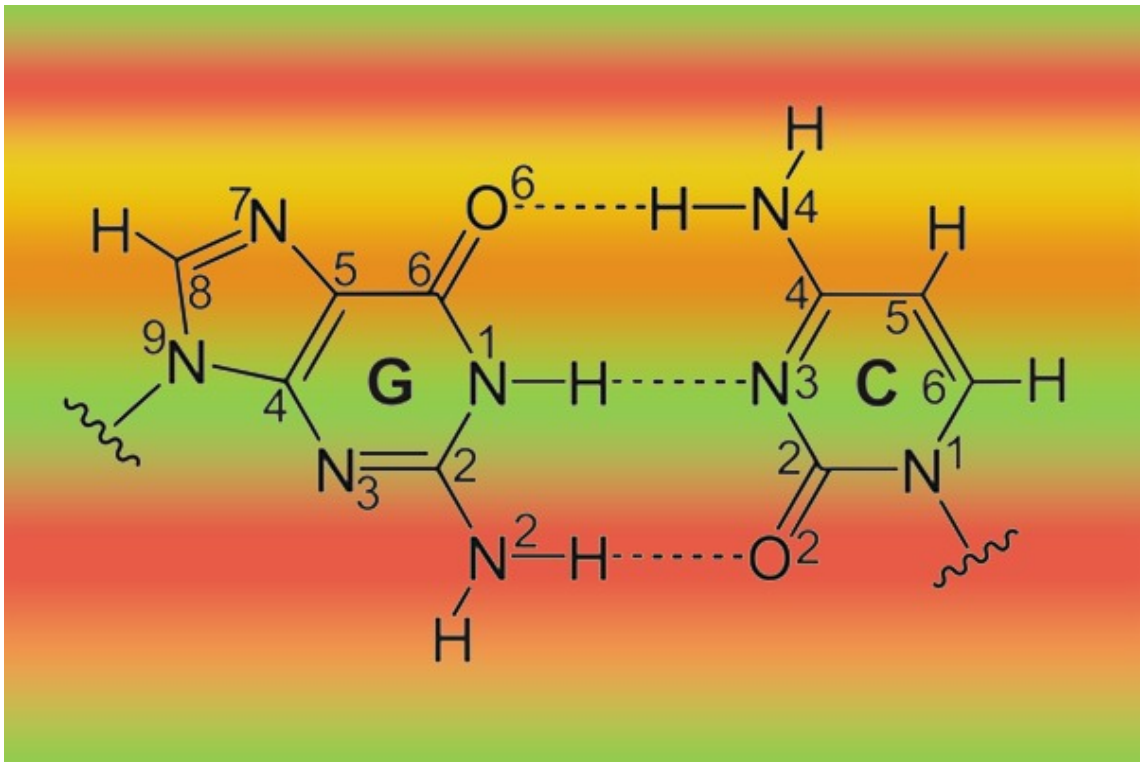
Finally, let me draw your attention to two important announcements. One is for the IUCr Congress in Prague next year and the other is for nominations for the new W. H. and W. L. Bragg Prize, to be given during the Prague Congress.

Original article: https://www.iucr.org/news/newsletter/etc/articles?issue=142706&result_138339_result_page=3

RESEARCH NEWS

Ideal bond lengths and angles in nucleic acid structures: an update for the 2020s

Andrew J. Howard



In the April 2019 issue of *Acta Cryst. B*, a toolkit for analysis of nucleic acid structures was reported by Mariusz Jaskolski and co-workers (Gilski *et al*., 2019). This paper is a valuable addition to the toolkit for analysis of nucleic acid structures. It alters the specific optimal values for bond-length and bond-angle restraint values in Watson–Crick base pairs. It also reduces the variability in those values beyond what is currently available, which are based on a study by Parkinson *et al*. (1996). The approach taken here, incorporating Cambridge Structural Database (CSD; Groom *et al*., 2016) structures, quantum-mechanical (QM) calculations and two ultra-high resolution nucleic acid crystal structures in the Protein Data Bank (PDB; Berman *et al*., 2000), provides a robust basis for both the ideal bond-length and bond-angle values and for the estimated variability in those values. The Parkinson study was based only on CSD structures available in 1996; the Gilski study has 10 times as many CSD structures from which to draw, and the authors are combining the CSD analyses with these other two sources of information. They provide tables of bond lengths and angles not only for CG and AT pairs, but also for the isolated bases, for an isocytosine–isoguanine base pair and for isocytosine and isoguanine alone. The authors subject the data to an elaborate statistical analysis that provides further justification for their values. They also inquire into whether the bond lengths and angles found in isolated bases differ significantly from those found in base pairs: the answer is that the differences are small but discernible.

The authors' QM calculations are based on nucleobases attached to methyl groups rather than on actual nucleosides or nucleotides. This simplifies the QM calculations significantly as compared with real nucleosides, and one can hope that that simplification will have little effect on the correctness or applicability of the data. The fact that the QM results are, for the most part, consistent with the CSD and PDB results provides additional confidence that their QM models are adequate. The accuracy of those QM results is poorer than the experimental results, but it remains reliable enough to be usable in situations where, as they state, 'no reliable experimental structural information is available.'

The authors base their analysis in part on two oligonucleotide structures available in the PDB, namely 3p4j, which is a CG-only Z-DNA structure determined at 0.55 Å resolution; and 1d8g, which is a B-DNA decamer containing all four bases, determined at 0.74 Å resolution. Both of these structures were determined without applying restraints on the bond lengths and angles in the final refinements, which justifies their scrutiny in a study of this sort. Neither of these structures incorporated charge-density analyses. The authors note that the bond lengths and angles in 3p4j are considerably more uniform than in 1d8g. This higher degree of regularity in 3p4j may arise because the structure was determined at somewhat higher resolution, as the authors suggest; but it may also show the influence of the narrower range of conformational heterogeneity available in a CG-only structure, or even because Z-DNA is perhaps more conformationally constrained than B-DNA. The authors' efforts here could inspire further analysis of other ultra-high resolution nucleic acid structures, to see whether the variability (or lack thereof) discussed in this study carries over into those other structures. There are now at least eight DNA structures and three RNA structures in the PDB that have been determined at better than 0.85 Å resolution. Several of these were refined with built-in bond length and angle restraints, which render them unsuitable for comparisons of this sort; but it would be straightforward to reanalyze those structures in the absence of those restraints, enabling this kind of analysis.

In general, though, this paper by Gilski *et al*. represents a significant step forward in providing statistically justifiable estimates for bond lengths and angles in nucleic acid structures, and should be consulted in the development of the next generation of software packages in encoding restraints.

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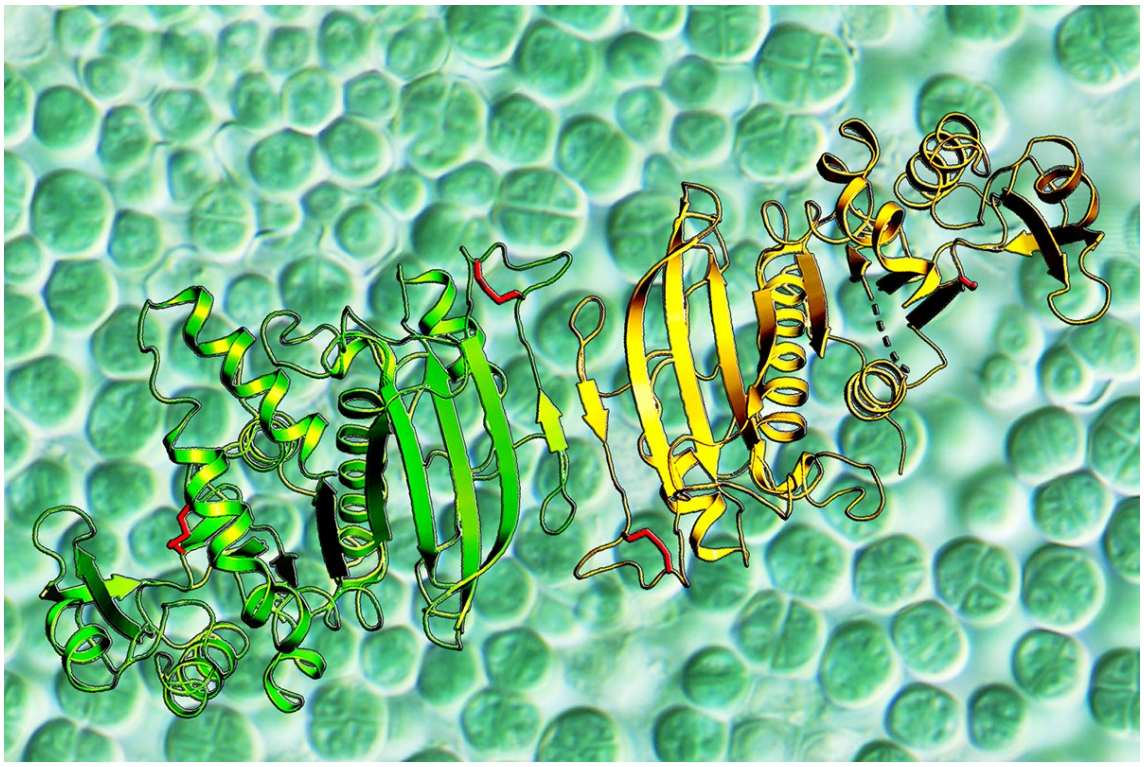
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Original article: https://www.iucr.org/news/newsletter/etc/articles?issue=142706&result_138339_result_page=5

RESEARCH NEWS

How photosynthesis gets turned off when the lights go out



In photosynthetic organisms, carbon fixation must be coordinated with the light harvesting reactions to prevent unnecessary energy expenditure in the absence of light. The enzyme phosphoribulokinase (PRK) produces the substrate for the carbon fixation step and switches off reversibly by disulfide bond formation. How this works in β-cyanobacteria is reported in a recent article in *Acta Cryst. F* by Wilson *et al.* (2019) and the Proteopedia molecular tour accompanying the article.

The paper describes the dimeric structure of PRK from the cyanobacterium *Synechococcus* PCC6301. This enzyme catalyzes the transfer of a second phosphate group onto ribulose 5-phosphate, thus creating the ribulose-1,5-bisphosphate (RuBP) substrate for ribulose 1,5-bisphosphate carboxylase/oxygenase (RuBisCO). The need for RuBP is found in virtually all autotrophic organisms, and there are corresponding PRKs in all kingdoms. Phylogenetic analyses of PRKs show two broad classes of enzymes, prokaryotic homo-octameric systems and thiol-regulated dimeric enzymes.

Dimeric PRKs are found in cyanobacteria, green algae and higher plants, and in these organisms the formation of a disulfide bridge across the active site effectively closes down the enzyme. The blocking disulfide is controlled by the local redox environment, which in turn is coupled to the ambient light levels. The formation of a cysteine disulfide bond in the absence of light blocks substrate binding. PRKs from green algae and plants contain a conserved insertion, which might add an additional layer of regulation in eukaryotes. In dimeric archaeal PRKs, this redox mechanism is not possible, due to the absence of the

necessary cysteine residues. Of note, β-cyanobacteria, algae and plants additionally shut down a second enzyme of the carbon fixation pathway, GAPDH, via complex formation with PRK and the adaptor protein CP12. CP12 also shows redox regulation, transitioning from an intrinsically disordered form into a structured oxidized form in the absence of light, which facilitates CP12's interaction with PRK and GAPDH. Structure determination of this inactive complex is pursued by the Murray Lab at Imperial College, London, UK.

Results of a parallel study are reported in a recent paper by Gurrieri *et al.* (2019), which presents the structures of a plant chloroplast PRK and algal PRK. These show the same pattern of cysteine arrangement poised for controlling the activity of the enzyme, but coupled with a longer 'clamp loop', postulated to bring the regulatory thiol side chains into proximity as needed.

Enzymes from simpler hosts are not necessarily simpler to work with: the prokaryotic enzyme crystallized and diffracted well, but in a system where molecular replacement was insufficient, it required the addition of data from an osmium derivative to unambiguously describe the second PKR monomer (Wilson *et al*., 2019). The very same molecular replacement model (PDB entry 5b3f; Kono *et al.*, 2016) was sufficient to solve the plant system (Gurrieri *et al.*, 2019).

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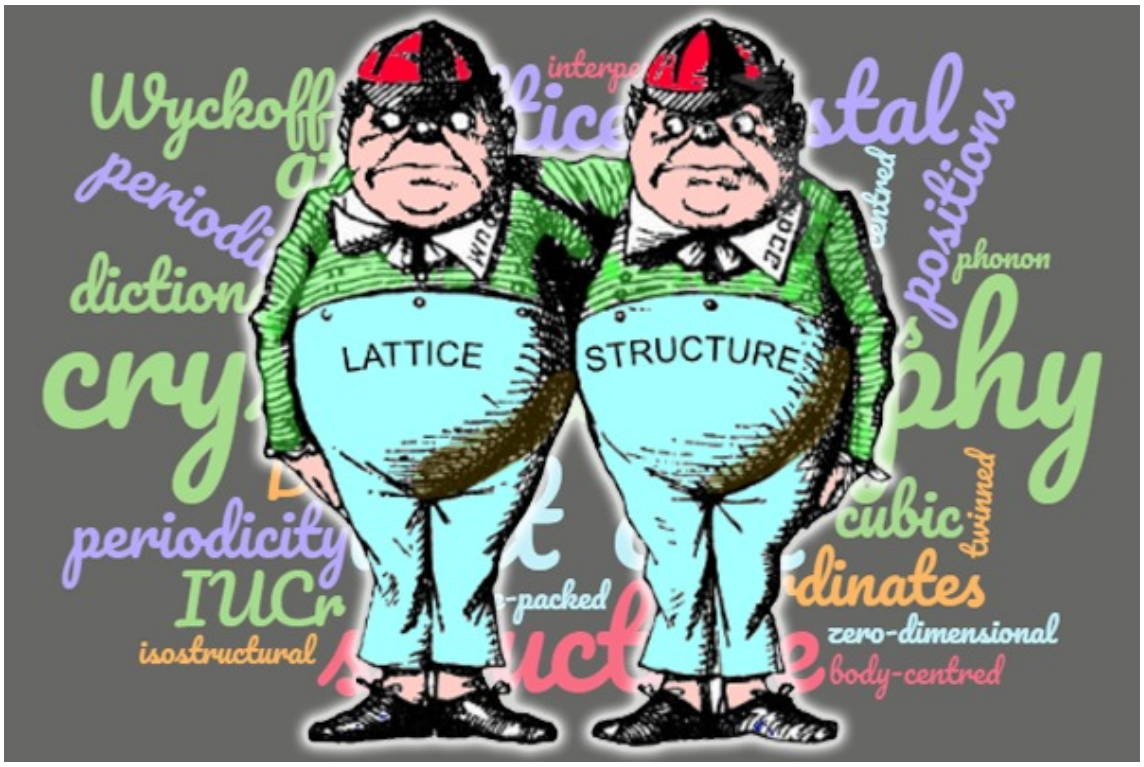
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Original article: https://www.iucr.org/news/newsletter/etc/articles?issue=142706&result_138339_result_page=6

FEATURE ARTICLE

The lattice sickness pandemic

Massimo Nespolo



One of the first and most fundamental concepts every crystallographer learns in their (scientific) infancy is that of *lattice*, *i.e.* an infinite set of geometric points (known as *lattice nodes*) that represent the translational symmetry of an ideal crystal. If one node is taken as origin, all the other nodes are obtained by applying to it all the vectors that represent a translation of the crystal pattern, *i.e.* a rigid motion that does not modify the orientation of any element of the crystal pattern. The number of possible lattices is always infinite. However, lattices obtained by translation vectors that are one-by-one parallel to each other and differ in their length define a single type of lattice. For example, there are an infinite possible number of face-centred cubic (f.c.c.) lattices, which all differ by the length of the basis vector **a**; they all correspond to a single *type* of f.c.c. lattice. In one-, two- and three-dimensional spaces there are one, five and 14 unique lattice types, respectively, which are universally known as Bravais lattice types (they could have been named "Frankenheim lattice types" if Moritz Ludwig Frankenheim hadn't earlier counted 15 instead of 14 types in three dimensions).

A lattice being infinite, crystallographers use a finite portion to represent it: the *unit cell*. This unit cell has only two requirements: to have lattice nodes at its corners, and to be able to reconstruct the whole lattice by translations parallel to its edges. These requirements allow a large (in principle infinite) number of choices for the unit cell; the description of the crystal structure and the Hermann–Mauguin symbol of the space group depend on this choice. Some choices are particularly convenient; one unit cell has the

same symmetry as the lattice (the conventional cell), another unit cell may be particularly useful to compare the structure of a related compound or of a polymorph; still another unit cell can be preferable for studying a twinned crystal; in the end, the “best” unit cell depends on the choice of the investigator. Some unit cells are so often adopted that they have come to be indicated by a letter, for the sake of brevity (*P*, *A*, *B*, *C*, *I*, *F*, *R*, *H*, *D*; the last two are much less often used, though). In some cases, one may find it advantageous to use a unit cell that does not have a special name (letter): in that case, the centring translation vectors are explicitly indicated when the cell is chosen, and in the rest of the publication the author simply uses a non-reserved letter (*e.g. X* has been used in the literature).

Whatever be the choice of the unit cell, the latter is like an empty box, a container that waits for its contents: the atoms. Indeed, the unit cell does not have an atomic nature, it is a geometric abstraction made up of zero-dimensional points. It goes without saying that the lattice described by that cell is a geometric abstraction itself. Once atoms take their place in the unit cell, and therefore in the infinite unit cells all obtained by the translations, one gets a crystal structure (often shortened just to “structure”); if one puts something else (drawings of flowers, birds, fishes *etc*.), the result is a crystal pattern, *i.e.* an extended network of (real or imaginary) objects that have the same periodicity as a crystal structure.

The reader may wonder why I am wasting so much space emphasising something that should be considered a *lapalissade*.[1] Unfortunately, the scientific literature is polluted by completely nonsensical uses of the term “lattice”, which makes this call for attention unexpectedly necessary. I have recently published an article in the Teaching and Education section of the *Journal of Applied Crystallography* that deals with the confusion between lattice and structure (as well as between periodicity and dimensionality), where I have discussed some examples taken from the recent literature. The purpose of this text in this *IUCr Newsletter* is to alert a larger number of readers who are probably unaware of the confusion and may be making the same mistake without even realising it. In the following I repeatedly quote Wikipedia and other online resources, not because I consider them to be a reference, but because the world wide web is today a primary source for so many readers who incorrectly think that if a term is used in many different places, then it cannot be wrong. Unfortunately, copying-and-pasting the same mistake does not make it less wrong. As William James stated, “There's nothing so absurd that if you repeat it often enough, people will believe it”.

Practically every reader has most likely met expressions like “lattice vibrations” (a geometric point does not vibrate; an atom does), “lattice energy” (how can a geometric point have some energy associated with it?), “lattice dynamics” (a geometric point does not evolve with time), “ionic lattice” (points cannot have an electric charge) and so on. What the writer has in mind is obviously the structure, but because of an incorrect shortcut, he calls it *lattice*. This bad habit has such deep roots that often one no longer recognises how meaningless the term being used is. The most representative example is probably that of *lattice energy*, defined as “a measure of the energy released when ions are combined to make a compound” (https://en.wikipedia.org/wiki/Lattice_energy), a definition that every chemistry student has to metabolise in their first year. Yet, it is sufficient to think for a few seconds to understand how self-contradictory it is. Indeed,

“when ions are combined to make a compound” the result is a ***structure*** so that what is measured or computed is a *structural energy*. Unfortunately, the term “lattice energy” is so profoundly rooted that any effort to correct it would certainly be a Cervantian battle against windmills. Let us declare ourselves satisfied if the readers and the authors realise they are facing a shortcut that, for historical reasons, would be hard to fix.

In much the same way, “lattice vibrations” is used as a synonym for phonon. The latter is defined as “a collective excitation in a periodic, elastic arrangement of atoms or molecules in condensed matter, like solids and some liquids” (https://en.wikipedia.org/wiki/Phonon). It is therefore self-evident that what vibrate are atoms, not geometric points. In this case, the much more suitable term ***phonon* does** exist and is extensively used as well. There is therefore absolutely no reason to forgive an aberration like “lattice vibration”: this expression must simply be banned.

“Lattice dynamics” is another absurdity that you can frequently meet. It is defined as “the study of the vibrations of the atoms in a crystal”, so that we have one more meaningless term used instead of the correct word “phonons”. The BBC bitesize website falls into the same type of trap, when it gives a definition of ionic compounds such that “[a]n ionic lattice is held together by strong electrostatic forces of attraction between the oppositely charged ions”. The reader may enjoy wandering among other masterpieces like lattice water, for example. There are even people pretending to produce lattice waves, or manipulate lattice strain to influence lattice thermal conductivity (energy transmission by means of pure geometry – not even Walt Disney would have had such an idea)! Even more eyebrow raising is to discover that some may actually want to try to *damage* a lattice. Time permitting, one may play a little game and harvest meaningless titles in publication databases: not recommended for those with a history of depression!

But what is the origin of this confusion? To track down the original sin that has damned crystallographers apparently without hope for redemption is certainly not an easy task. Without any pretension at divination, one may make an educated guess by considering the simplest yet exceptional cases of crystal structures in which atoms occupy positions that coincide with lattice nodes. The cubic close-packing of spheres corresponds to a crystal structure in a space group of type *Fm*3*m* with spheres at the origin ($x = y = z = 0$) and at the centre of each face (two of the fractional coordinates ½, the third 0). This corresponds to Wyckoff position 4*a* and also to the fractional coordinates of the lattice nodes when the lattice is described by the conventional (*F*) unit cell. Therefore, the cubic close-packing (c.c.p.) is also called the face-centred cubic (f.c.c.) ***structure*** whose ***lattice***, needless to say, is face-centred cubic as well. Yet, the two concepts are by no means equivalent: the structure is made of atoms, and a number of metals crystallise in this type of structure (Ni, Cu, Ag, Au, Pt, Ir, Rh, Pb, Th, Ac), the lattice of geometric points, and in this specific case the atoms are on the positions of lattice nodes. A similar case is that of b.c.c. for the body-centred cubic structure *and* lattice. A number of metals crystallise in the b.c.c. structure type (V, W, Ta, Cr, Mo, Nb, Mn, Eu, Ba), which correspond to space groups of type *Im*3*m* and atoms with coordinates (0,0,0) and (½,½,½), *i.e.* Wyckoff position 2*a*. These are also the coordinates of lattice nodes when the lattice is described by the conventional (*I*) unit cell. These extremely simple yet very special cases are often used in textbooks to introduce crystal chemistry. Unfortunately, a clear distinction between lattice nodes and atomic positions is often missing and the student is misled into

believing that the concepts coincide. A clear example is that of the CsCl structure, which is *primitive* cubic: one type of atom sits on the origin, the other at the centre of the unit cell, but the two atoms being different there is no translation vector relating the two positions as is instead the case for the b.c.c. structure. CsCl crystallises in a space group of type *Pm*3*m*, with one atom in position 1*a* and the other in position 1*b*. Yet, a number of textbooks and online resources describe CsCl as "cubic centred", as if the chemical difference between the atoms could be ignored.

The situation starts getting more confused in the case of the diamond structure, which crystallises in a space group of type *Fd*3*m* with carbon atoms in Wyckoff position 8*a*: for origin choice 1, the coordinates in the asymmetric unit are 0,0,0 (they become ⅛,⅛,⅛ for origin choice 2). Now, the multiplicity of the Wyckoff position is 8, which means that there are eight atoms in the unit cell, whereas the *F*-centred unit cell contains only four nodes. This difference should be sufficient to avoid any possible confusion. Yet, because there are none so blind as those who will not see, the structure of diamond is often described as "two interpenetrating face centered cubic Bravais lattices". Now, if one imagines taking an f.c.c. lattice $\mathbf{L}_1$, making of copy of it (let it be lattice $\mathbf{L}_2$) and moving the latter with respect to the former by ¼ along one of the body diagonals, the translation vectors of the resulting construction, which define the lattice, connect two nodes of $\mathbf{L}_1$ or two nodes of $\mathbf{L}_2$: the lattice is still $\mathbf{L}_1$. A vector connecting a node of $\mathbf{L}_1$ and a node of $\mathbf{L}_2$ does not extend beyond those two nodes, *i.e.* it does build up a periodic distribution of nodes, the definition of which is a lattice. If one instead takes an f.c.c. *structure* $\mathbf{S}_1$ (*e.g.* the structure of Ni: Figure 1a), repeats the process above to obtain the structure $\mathbf{S}_2$ and moves $\mathbf{S}_2$ by ¼ along one of the body diagonals of $\mathbf{S}_1$, the result is a new structure (Figure 1b): the sphalerite type of structure, or the diamond-type of structure if the two types of atoms become one (*i.e.* if one ignores the colour difference). Needless to say, Ni does not crystallise in this of type of structure; but if we replace Ni with C (the cell parameters are modified accordingly) we do get the structure of diamond. Both metallic Ni and diamond have a lattice of type f.c.c., but they have a different types of space group: *Fm*3*m* the former, *Fd*3*m* the latter (Figure 1). Interpenetrating two lattices does not make any sense: interpenetrating two structures does.

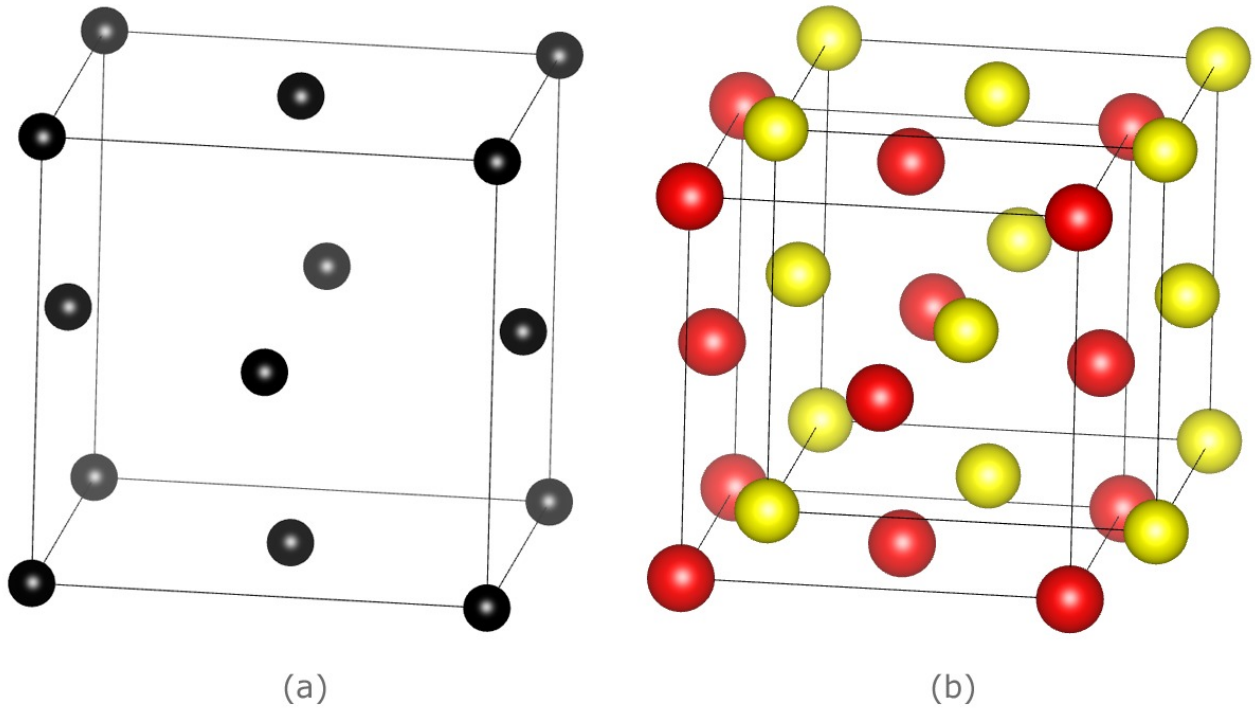


Figure 1. (a) An f.c.c. lattice, as well as the structure of metallic nickel, in which Ni atoms occupy the positions of lattice nodes. (b) Two copies of the structure of nickel, one in its original position (red), the other shifted by ¼ along one of the body diagonals (yellow). The colour difference is used simply to emphasise the logical process of constructing the new structure.

The result is isostructural to sphalerite, ZnS, or, if the colour difference is ignored, to diamond. Despite the 1:1 correspondence between the atomic positions and the positions of the lattice nodes in the case of metallic nickel, the atomic nature is fundamental in constructing a new, derivative structure: to move lattice nodes does not make any sense.

Even worse is the case of the hexagonal close-packed structure, which corresponds to space groups of type $P6_3/mmc$ and atoms with coordinates ⅔,⅓,¼ and ⅓,⅔,¾ (Wyckoff position 2*d*) or ⅓,⅔,¼ and ⅔,⅓,¾ (Wyckoff position 2*c*) *i.e.* away from the lattice nodes, yet the meaningless term *hcp lattice* is frequently used.

Finally, why does all this matter? Is this just pedantry? Well, for a start, terms like *lattice* and *structure* have been defined on an international basis by the IUCr, in much the same way as most other physical terms are. For instance, we would not be allowed to use, say, *g* the acceleration due to gravity, as the same as the *force* due to gravity. Or, for example, *energy* when one means *entropy*. And so on. The reason for the importance of using correct terminology is to enhance communication and ensure that different people do not end up talking at cross purposes.

Paraphrasing Zizi's Lament,[2] so many authors may today sing "I am in love with the lattice sickness ...".

Notes

1. A truism.

2. From Gregory Corso’s text for Leonard Bernstein’s *Songfest*: "I am in love with the laughing sickness ...".

Original article: https://www.iucr.org/news/newsletter/etc/articles?issue=142706&result_138339_result_page=7

FEATURE ARTICLE

Indiana Jones and the Crystal Skull

Juan Manuel García-Ruiz



I like the Indiana Jones films. Ever since the first ark-full of surprises, each movie has absorbed me so much that I haven't even touched the popcorn – although the latest instalment did leave me with a bitter taste in the mouth. Yet here I am not going to write about *Indiana Jones and the Kingdom of the Crystal Skull* (Frondel, 1966), but about the crystal of the skull.

In Romance languages, when you speak of "crystal", most people think of glass windows, bottles or spectacles, and in English there is a related confusion with "crystal glass". This is inherited from the Romans, who used transparent sheets of gypsum crystal in their windows. Back then, this gypsum was called *Crystal of Hispania* because it was extracted from the mines of Segobriga (modern-day Cuenca) in Spain. When plate glass was invented, Segobriga's commerce collapsed, but the sheets of glass that replaced Hispania crystal continued to be called crystal. Hence the confusion.

Salvador Dalí once said that the difference between the best photograph of the *Juan de Pareja* and the actual Juan de Pareja portrait painted by Velázquez was exactly five million dollars. To paraphrase this brilliant artist, we can state that the difference between a carbon crystal – that's to say, a diamond – and a piece of amorphous carbon is exactly the fortune that the diamond is worth. This is because, unlike the internal disorder of amorphous glass, the perfect order of the atoms inside a diamond crystal is what gives it its properties.

The skull from Indy’s latest adventure is made of quartz, a fascinating crystal of silicon oxide (Frondel, 1966; http://www.imdb.com/title/tt0367882/?ref_=sr_2; https://en.wikipedia.org/wiki/Quartz). If you make a circuit with a pair of copper wires, a small light bulb and a quartz crystal, and press the crystal firmly, the bulb will light up because the electrical charges of the crystalline structure move around, creating a voltage, briefly turning the crystal into a battery. This is how a gas lighter works: it carries a small quartz crystal, which, when struck sharply, generates an electric arc, a spark that – zap! – ignites the gas. Conversely, if an electric current is applied to the quartz crystal, it is imperceptibly deformed, and when the current is removed the crystal recovers its initial shape. If this is done in water, these elastic deformations of the crystal create a wave that spreads out until it hits another object, for example a submarine or the seabed, and the wave that bounces back deforms the quartz crystal again, which generates an electrical signal. If you measure the time the wave takes going out and back, you can learn how far away the seabed or the submarine is. Sound familiar? Yes, this is the sonar that ships use. This is also how oscillators, microphones and the pickups on electric guitars work. Furthermore, if you apply the electric current in pulses, the quartz crystal goes into resonance, as a tuning fork does, producing a frequency that is inaudible but so precise that it is used to regulate clocks and watches (http://www.quartzpage.de/index.html). You can read more about this so-called piezoelectric effect in the *IUCr Newsletter* (see https://www.iucr.org/news/newsletter/volume-26/number-2/some-musings-on-crystals-of-quartz). These are only a small sample of the properties of the quartz crystal ("The Quartz Watch – Inventors". The Lemelson Center, National Museum of American History, Smithsonian Institution. Archived from the original on 7 January 2009), added to which is the exquisite beauty of any of its varieties: the episcopal violet amethyst, the lemon-yellow citrine, the enigmatic smoky quartz or the limpid rock crystal. Some people, not content with all this, insist on attributing curative powers, magical properties, mysterious energies and whatnot to quartz, all of which are nonsense, but among them are those behind the entertaining little story of the skulls in the Indiana Jones film.



The enigma surrounding the crystal skulls is how such a perfect skull could have been carved in pre-Columbian times. The most famous and enigmatic skull was allegedly discovered in 1924 by Anna Mitchell-Hedges, adopted daughter of British adventurer and popular author F. A. Mitchell-Hedges (for more details see https://en.wikipedia.org/wiki/Crystal_skull).

Quartz crystals do not have preferred directions for carving (contrary to what is said in the film). Rather, when they are struck they break into concave pieces, just as glass does. They are thus easy to work with, despite their hardness, and polish well using the dust from quartz itself. In fact, the Romans, Greeks and Mayas created wonderful small carvings of rock crystal with the rudimentary tools they then had available. The making of the natural-sized “pre-Columbian” skulls, however, is more difficult to explain. Above all, if the fact that they are not truly pre-Columbian is concealed, then how can we know? Now, another fantastic property of quartz is through its thermoluminescence. It turns out that if you irradiate a quartz crystal, it creates defects in its structure. When the crystal is heated, the structure relaxes these defects, emitting light – the more light the more it has been irradiated. This is how the dosimeters used by hospital staff who work close to radiation sources function. In nature, cosmic rays are the sole source of irradiation, so if you heat a crystal quartz you can find out how long it has been exposed to those rays – that is, you can find out how old it is. Thus, we are able to detect that the crystal skulls were made no more than a century and a bit ago, with modern carving technology. In other words, they are a fraud (see https://www.iucr.org/news/newsletter/volume-27/number-1/more-fun-with-quartz-crystals!). But let us not let the truth spoil a good story! So let’s suppose that the crystal skulls were made 3000 years ago. If the indigenous peoples did not make them, then who did? Of course! The only possibility can be that they

were the work of extraterrestrial beings that visited the Incas, Mayas or Aztecs in order to pass on their knowledge and power. I find this absurdly difficult to believe, because every time I try, the ghost of a disbelieving Aztec appears before me – there have always been non-believers – prostrate in the ruins of Tenochtitlan, cursing his gods and muttering, “all those lasers, all that high technology, all that crystal skull and such…. If those alien morons had shown us the wheel then we really could have shown those bearded invaders from across the pond what an obsidian blade is worth!”

As there is so much talk about the magic of crystals, I promise some time to write about it. But let me emphasize that if you are seeking mineral crystals with power, the only ones that are truly powerful are diamonds and emeralds. Believe me. Word of a crystallographer.



Why have I chosen this film for the teaching of crystallography?

You may wonder why I have chosen this film for a series on crystallography and cinema. The reason is twofold: first, because it is an excellent film that is about a skull made out of rock crystal, also termed quartz; second, because it employs the crystal as an object with magical powers, making use of that historical and universal tendency to believe that crystals possess a mysterious energy with beneficial healing powers.

This is a good occasion to counterpose the supposed magical powers of crystals with the even more fabulous properties that quartz crystals actually have. The physical properties of crystals are just as wonderful as the supposed magical properties that so-called healers, shamans and charlatans claim for crystallomancy (belief in the capacity of crystals to foresee the future and change fate).

Suggested reading and further information

The investigation scientifically revealing the fraud of the false Mesoamerican crystal skulls, which is the story the film is based on, can be found in the article by J. M. Walsh (2008).

A good summary of the properties of quartz is the article in Wikipedia on this mineral: https://en.wikipedia.org/wiki/Quartz. Another excellent website on quartz is http://www.quartzpage.de/index.html.

I also encourage teachers to use the website of the exhibition CRISTALES "A WORLD TO DISCOVER" (http://www.cristallografia.org/contenuto/articolo-cristales-a-world-to-discover-an-exhibition-for-schools-and-universities-ad-accesso-libero-su-j-appl-cryst/773), which is written in English and Spanish. On this website, students will find information about crystals and their properties, as well as about crystallographic methods. The posters and panels of the exhibition can be freely downloaded to be displayed in schools and universities.

A link to the Indiana Jones film's technical specifications on IMDB can be found here.

Part of this article is an English translation of an extract from the *Guía de la Cristalografía en el cine* by Juan Manuel García-Ruiz and Martha Santana. This guide can be downloaded from Fundación Descubre at https://clickmica.fundaciondescubre.es/files/2017/02/guiacristalografia.pdf.

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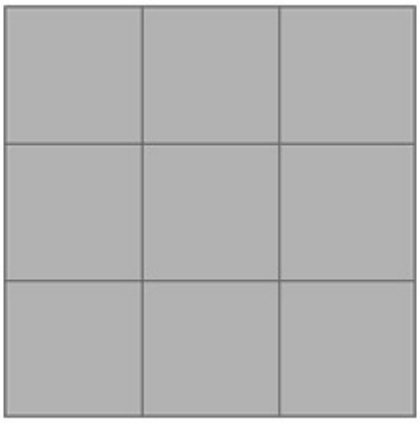
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Original article: https://www.iucr.org/news/newsletter/etc/articles?issue=142706&result_138339_result_page=8

FEATURE ARTICLE

Auxetics: Don’t Pull Me, I’ll Get Fatter!

James-N Grima-Cornish



The use of materials is one of the main pillars that has led to humankind’s success. The evolution of the materials we use to manufacture tools, products and structures has allowed for the innovation of more advanced creations, and hence, further advancements of humankind itself. In more recent years, as knowledge of materials having so-called “regular” properties has increased, scientists and engineers gradually began to focus their attention on materials with properties termed “irregular” or anomalous. Anomalous properties are of great interest, leading to a number of possible and previously unattainable modern applications.

Anomalous properties can be divided into (i) anomalous electronic properties, relating to the properties associated with electrons and their interactions; (ii) anomalous structural properties, which refer to properties arising from the arrangement of atoms, grains and other building blocks of a material; and (iii) anomalous mechanical properties, which refer to the response of a material when applying mechanical loads. While both (i) and (ii) are significant subjects of interest in their own right, here we shall focus on an important anomalous mechanical property, namely auxeticity. It should be noted, however, that even though anomalous properties can be divided into categories, we should not assume that there is no “bridging” of one type of property to another. In fact, auxeticity is highly reliant on the structure/geometry of the material, even though it is considered to be a mechanical property.

Auxeticity, a term coined by K. E. Evans and coworkers in 1991 (Evans *et al.*, 1991), can be defined as the material property of having a negative Poisson’s ratio. A visual example of auxeticity is given in Figure 1, which shows how auxetic materials become “fatter” when uniaxially stretched and “thinner” when uniaxially compressed.

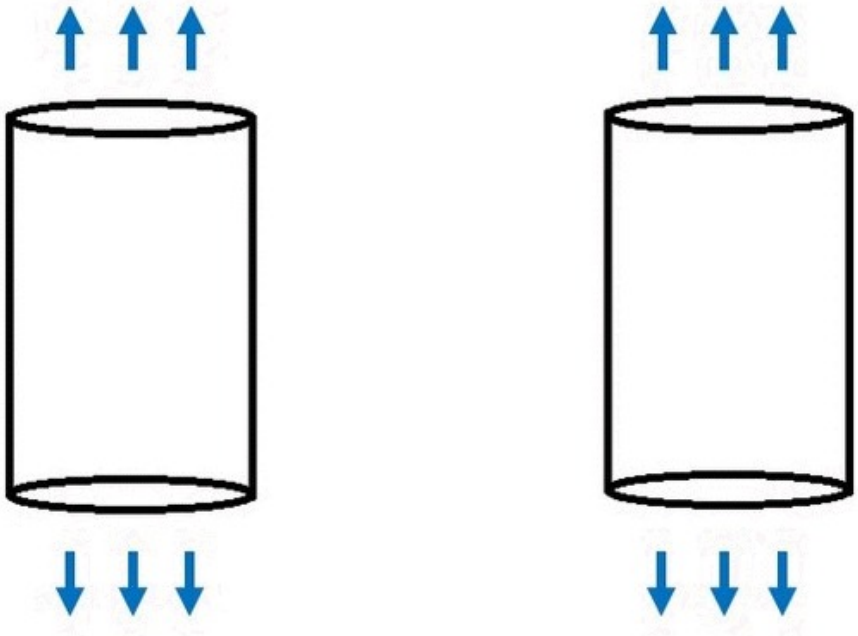


Figure 1. (Left) a material behaving in an auxetic manner when uniaxially stretched/compressed, and (right) a material behaving in a conventional manner when uniaxially stretched/compressed.

In order for a material to be auxetic, it must have particular geometric features as well as an amenable deformation mechanism that permits the 'geometry' to deform in a fashion that allows for auxetic behaviour to be exhibited. The combination of the two required features creates what can be termed as 'auxetic mechanisms', a grouping made in order to simplify the matter, with applicability of these mechanisms in various real situations ranging from natural and synthetic materials, such as crystals or giant nanonetworks, to giant architectural constructs.

There are two main categories of auxetic mechanisms: *stretching,* whereby structural elements lengthen or slide past each other, such as triangular structures made of ligaments analogous to shock absorbers (Rothenburg *et al.*, 1991) and two-dimensional models of hexagonal molecules on a hexagonal lattice interacting via a nearest-neighbour *n*-inverse-power site (Wojciechowski, 1987); and *rotation,* whereby internal units rotate relative to each other such as in the rotating squares mechanism (Grima & Evans, 2000), re-entrant honeycomb mechanism (Kolpakov, 1985) and nodule-fibril mechanism observed in certain polymeric materials (Evans & Alderson, 2000).

Stretching mechanisms, as noted above, are all mechanisms leading to auxeticity that can be attributed to the lengthening of structural elements or sliding of elements past each other. An auxetic mechanism of this type is Rothenburg *et al.*'s (1991) triangular structures made of ligaments that are analogous to shock absorbers (see Figure 2, left). Here, when applying a uniaxial stress to the structure made of ligaments in any direction, the deformation that occurs causes a reduction in the length of all three units as a result of the shock-absorber-like units present. Another mechanism for auxeticity based on a stretching mechanism is Wojciechowski's (1987) two-dimensional models of hexagonal

molecules on a hexagonal array interacting via a nearest-neighbour *n*-inverse-power site–site potential (see Figure 2, right): a system that becomes auxetic at high densities because of the repulsion between atoms within the hexagonal system.

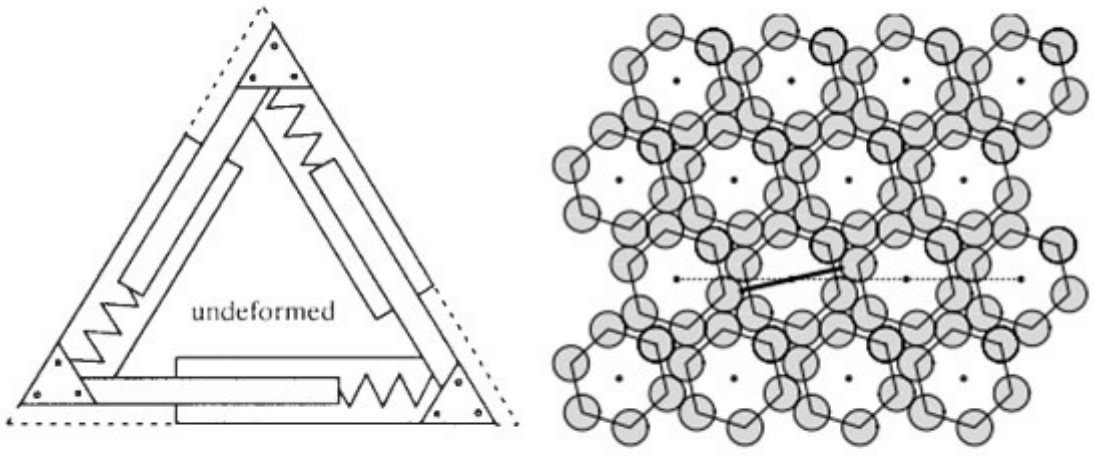


Figure 2. Stretching mechanisms leading to auxeticity, specifically Rothenburg *et al.*'s (1991) hexagonal auxetic structure made of ligaments that are analogous to shock absorbers (left); and Wojciechowski's (1987) two-dimensional models of hexagonal molecules on a hexagonal array interacting via a nearest-neighbour n-inverse-power site–site potential (right).

More commonly, auxeticity in materials can be attributed to a rotating mechanism that, as noted above, involves the rotation of units relative to each other. Before proceeding any further it should be noted that rotations can also be described in terms of micro-domain changes, rather than simply rotations of a rigid unit around a point, such as in defective graphene. In three dimensions, rotating mechanisms for auxeticity include rotating polyhedra mechanisms. These systems involve rotations of rigid/semi-rigid polyhedra in a manner that results in the elongation in one direction or more when "pulling" the structure, and a reduction in one dimension or more when "pressing" the structure (in particular directions). Such 3D mechanisms have been applied at both the macroscale [*e.g.* in the structure suggested by Attard & Grima (2012), shown in Figure 3 (left)] and the nanoscale, including crystal structures such as α-cristobalite shown in Figure 3 (right) (Alderson & Evans, 2001).

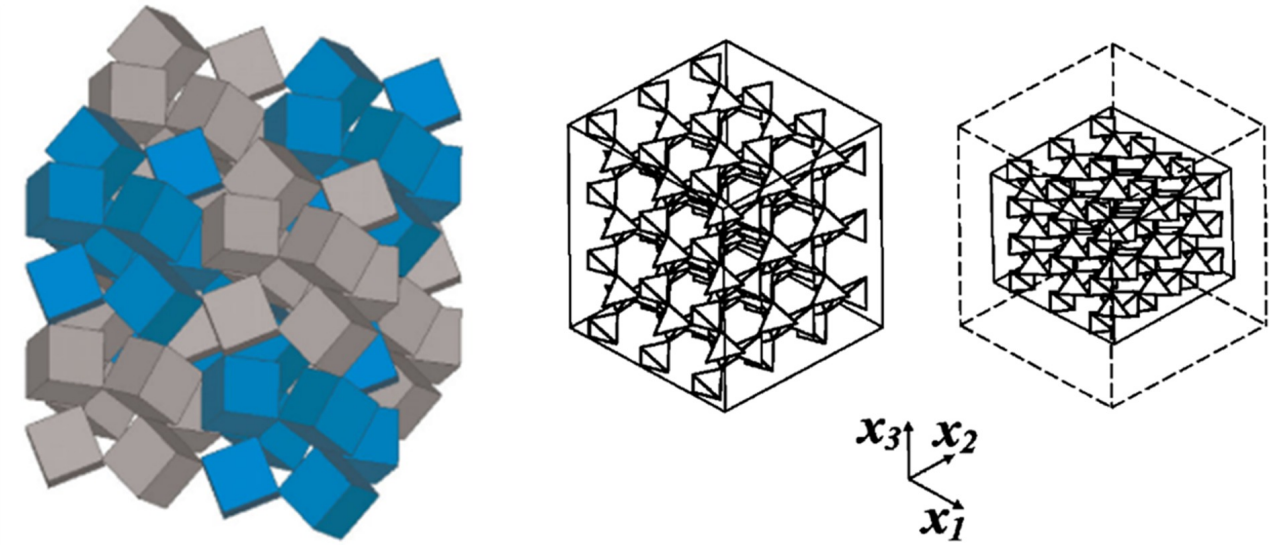


Figure 3. (Left) connected cuboid structure suggested by Attard & Grima (2012). (Right) rotating tetrahedral model by Alderson & Evans (2001).

Unfortunately, 3D auxetic models can sometimes be rather complex to conceptualise and, as a result, a number of simpler yet equally effective 2D models have also been proposed to explain the auxeticity in materials. In this category, we find mechanisms that are generally referred to as rigid/semi-rigid rotating polygon mechanisms. Because of the high incidence of manifestation in crystal structures when viewed in particular planes, this discussion will be focused on the rotating square/rectangle mechanisms which exhibit a Poisson's ratios of –1 for loading in any direction (see Figure 4, top). These mechanisms and others such as the rotating triangles mechanism, which have their own applicability, may be regarded as "perfect" auxetic systems, demonstrating auxeticity when stress is applied in any direction. Such perfection is difficult to achieve in real systems such as crystals or foams, and it has been shown that when the polygons in the structure are no longer rigid but semi-rigid, the Poisson's' ratio increases from its ideal value of –1, making the structure less auxetic and anisotropic. Such semi-rigid rotating polygon models have been used successfully to explain the auxeticity in various systems including crystals such as α-cristobalite, which can be considered to have a semi-rigid rotating rectangle mechanism in particular crystal faces, as discussed by Grima *et al.* (2006); Thomsonite (see Figure 4, bottom); natrolite; and a number of others.

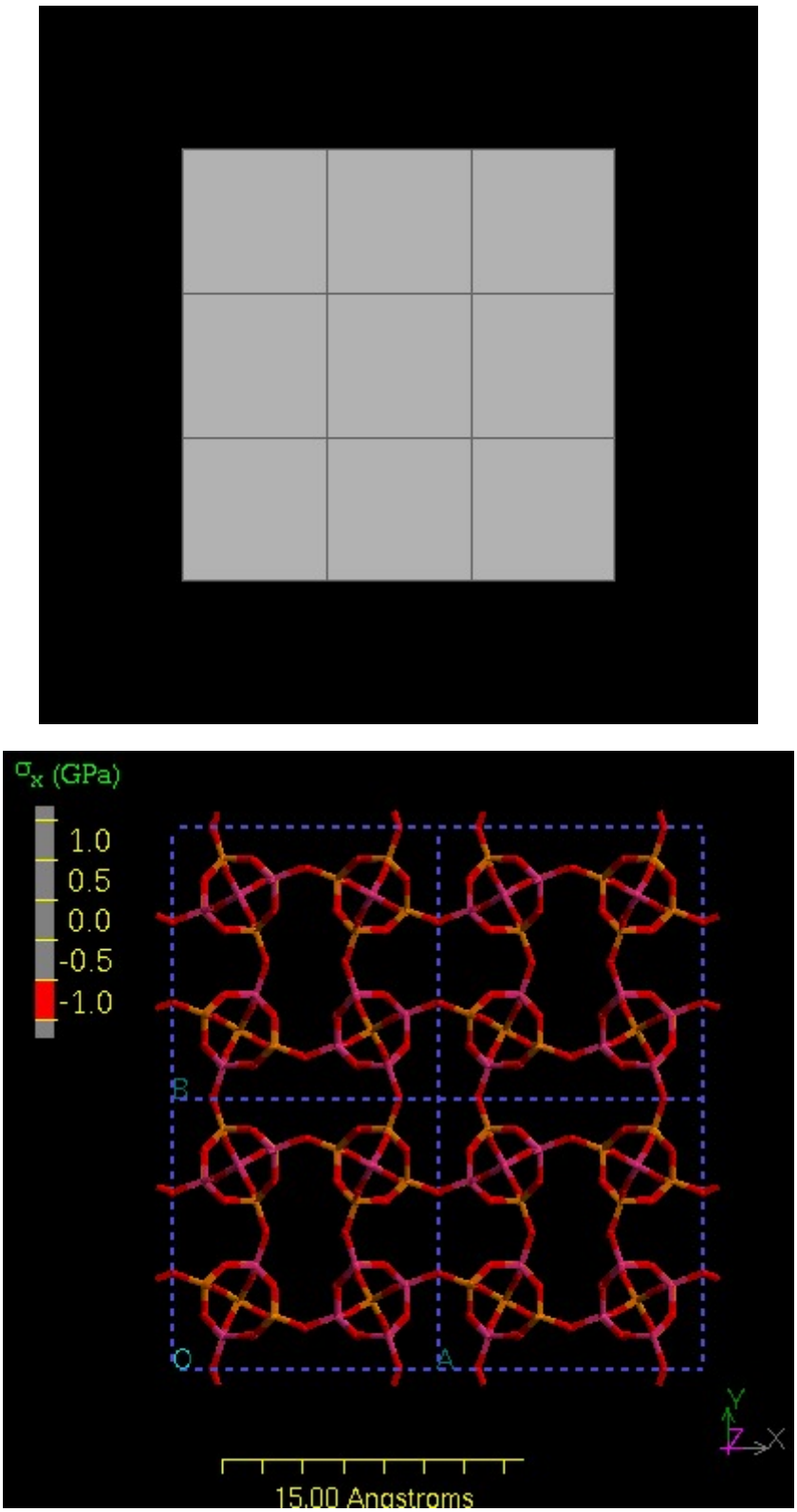


Figure 4. (Top) the rotating squares mechanism. (Bottom) the rotating squares mechanism observable in Thomsonite.

Another important 2D mechanism that may feature in materials when viewed in two-dimensional space is the "*wine rack*" mechanism, where rigid ligaments (which can be considered as the one-dimensional equivalent of polygons) rotate relative to each other in a manner resulting in the wine-rack 'opening'. The opening of this structure occurs when applying uniaxial stress in certain off-axis directions. If the stress were to be applied on-axis this effect would not be observed, as the structure would deform in a manner to

maximise elongation in the direction of loading, and the structure begins to close (Caruana-Gauci *et al.*, 2018). This highlights the anisotropy possible for such a material property. Similar to the wine-rack mechanism for auxeticity described above is the 2D re-entrant honeycomb mechanism. This is also composed of rigid ligaments considered to be the one-dimensional equivalents of polygons rotating relative to each other. Upon the application of uniaxial stress in particular directions, the re-entrant structure begins to expand as shown in Figure 5, with a negative Poisson's ratio being observed until the structure takes the shape of "rectangles" or "squares". At the point of achieving this "squareness", the Poisson's ratio becomes positive upon further application of stress. This structure is also anisotropic.

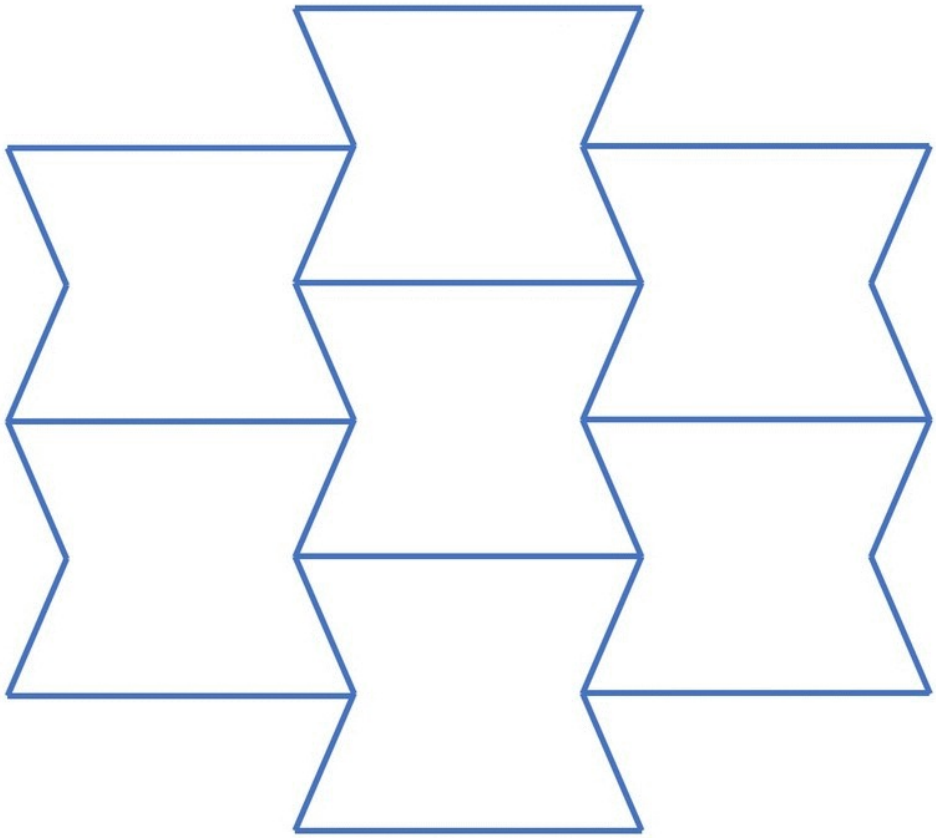


Figure 5. Re-entrant mechanism for auxeticity in action. Note how it reaches the described structure composed of "squares".

Applications of materials with anomalous properties are vast and always growing, including those of materials that exhibit auxeticity. This can be attributed to the fact that certain applications that could not be achieved previously using materials with "regular" properties are now possible because of these "irregular" properties. This statement is true on the macroscale, *i.e.* materials above the microscale (>0.1 mm), which can usually be viewed by the naked eye; the microscale (0.001–0.1 mm); and the nanoscale (<0.001 mm), as auxetic materials have been considered and applied in applications down to the smallest of sizes.

On the macroscale, applications of auxetic materials and structures include sportswear applications, clothing, furniture, yarns, protection and home improvement. A recent push has also been made towards auxetic architecture, where these materials – owing to the versatility of these structures, their aesthetics and a number of other reasons – are being applied to structures such as the Munich 1972 Olympic Park roof shown in Figure 6 (right), which can be likened to the opened re-entrant structure shown in Figure 6 (left). In the future, such domes could possibly be constructed by the application of auxetic structures in order to reduce time, equipment and materials required to erect these impressive buildings.

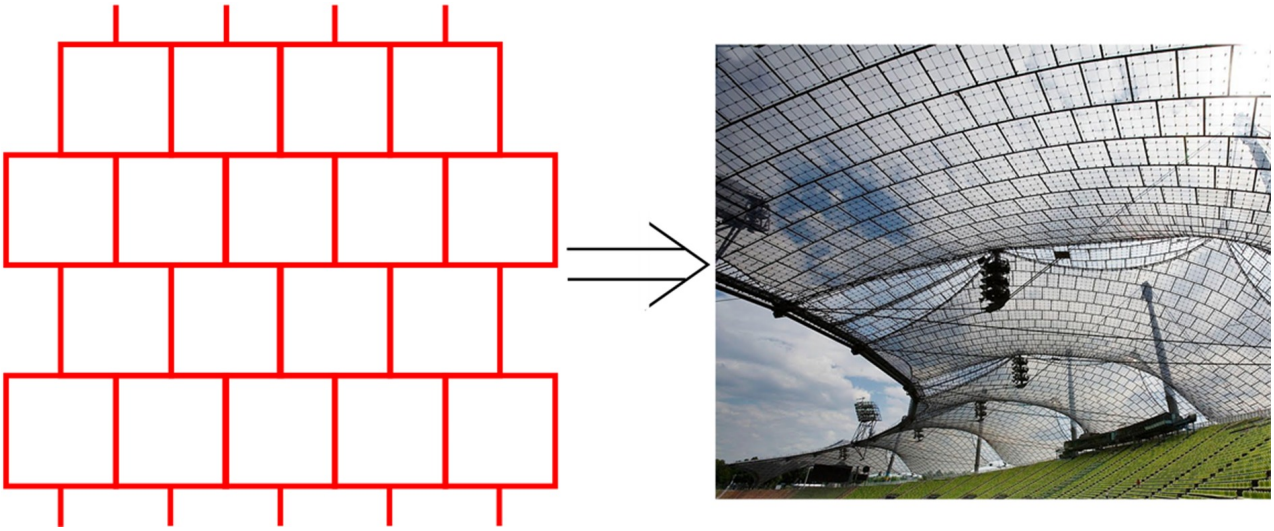


Figure 6. (Left) the opened re-entrant structure described above alongside (right) the Munich 1972 Olympic Park roof.

Auxetics in sportswear is currently an interesting field because of the anomalous ability of these structures to “dome”, and therefore take the shape of the subject (*e.g.* the sole of a foot) better than conventional materials. This can be seen in certain Nike shoes within the Nike Free collection, which use an auxetic sole [see Figure 7(a)], incorporating auxetic geometry consisting of a hexagonal array of triangles [see Figure 7(b)] in order to enhance the running experience; and in those in the Under Armour ClutchFit^{TM} collection, which have an auxetic upper (see Figure 8) for a "glove-like fit and feel that’s truly customized to every foot", which incorporates a number of different mechanisms throughout their range, including the re-entrant mechanism (see Figure 8, top) and the "arrowhead" mechanism (see Figure 8, bottom).

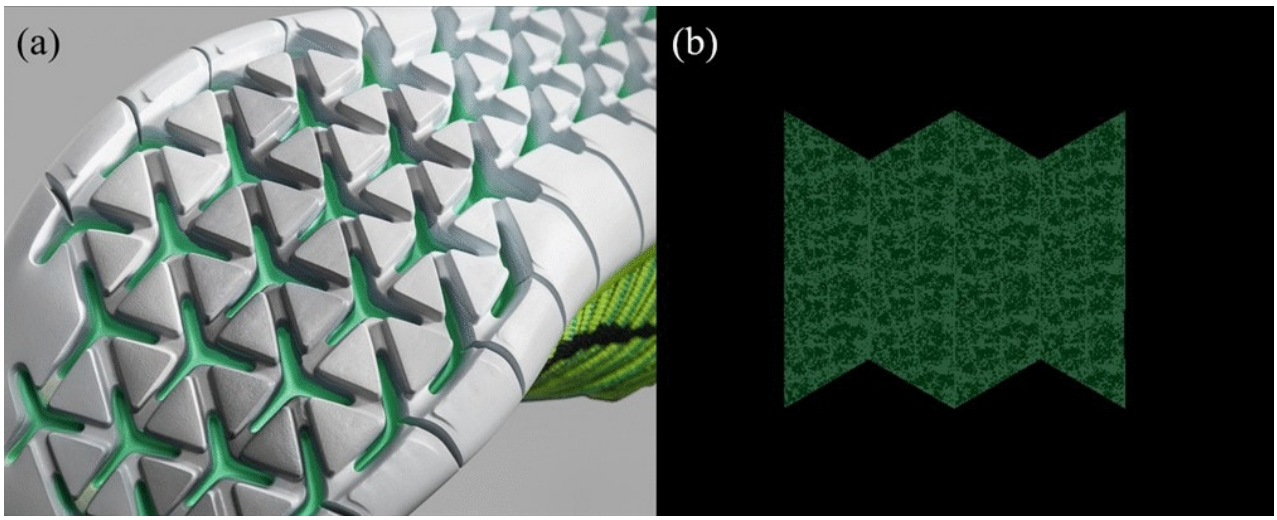


Figure 7. (a) Nike Inc.’s Free sole alongside (b) the auxetic array of incorporated triangles.

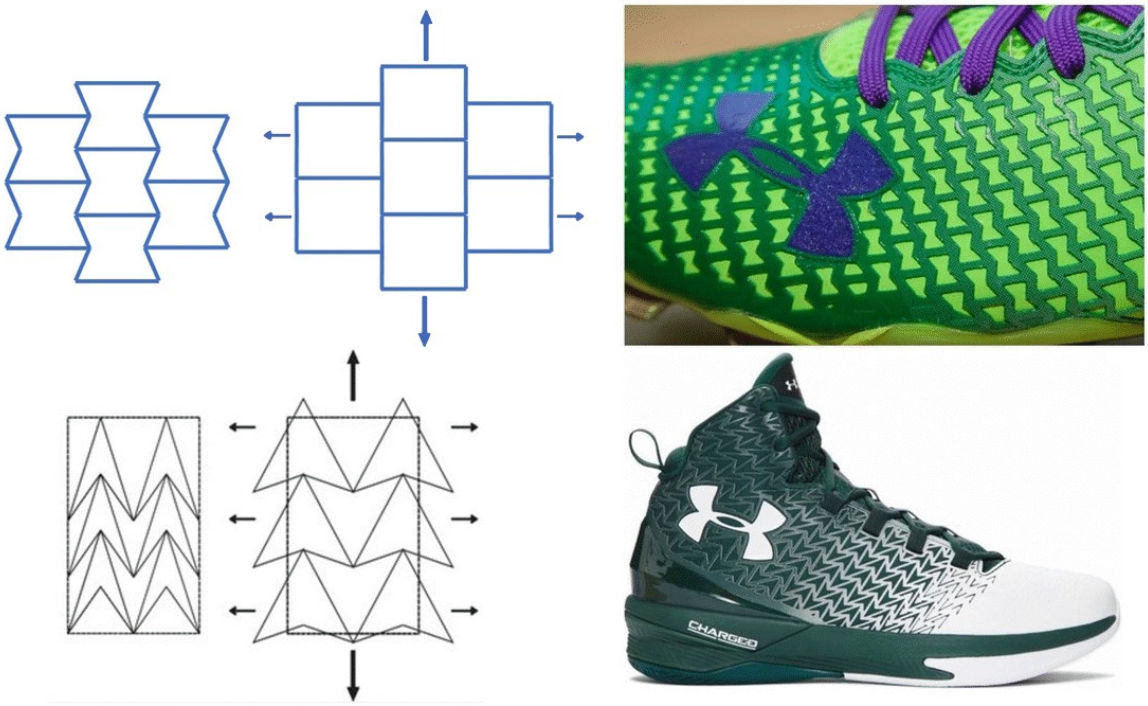


Figure 8. (Top) the idealised representation of the re-entrant mechanism alongside Under Armour Inc.’s ClutchFit, incorporating the re-entrant mechanism on the upper. (Bottom) the idealised representation of the arrowhead mechanism alongside Under Armour, Inc.’s ClutchFit, incorporating the arrowhead mechanism on the upper.

Auxetics have also been suggested and sometimes applied to clothing for both aesthetic and practical reasons. Apart from the obvious aesthetic reasons, they have a couple of advantages over classical textiles. For example, the auxetic clothes designed and manufactured by Petit Pli Ltd have the ability to adjust to the body’s natural contortions better and “grow” with the individual. These may be particularly appealing to pregnant women and growing children, as seen in Figure 9.

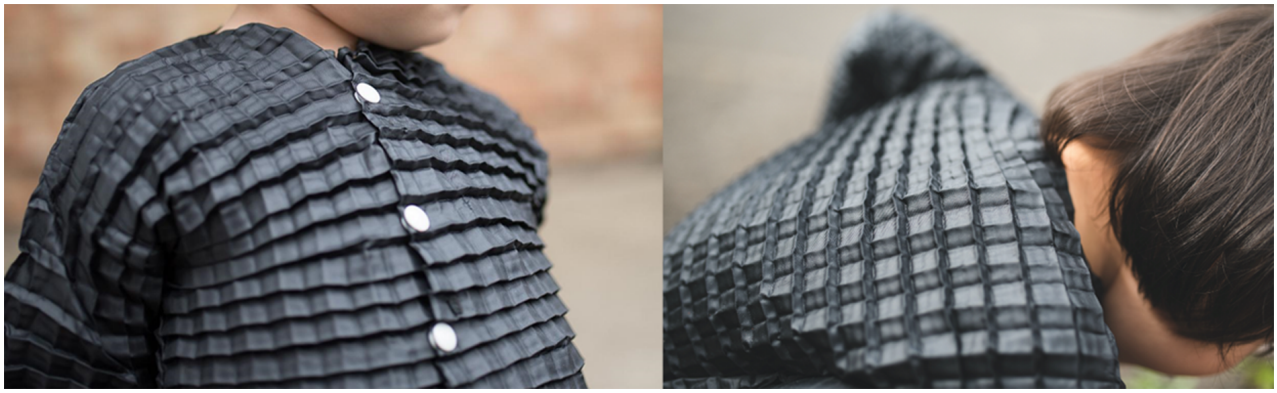


Figure 9. Auxetic clothing for children, which “grows” alongside their growth, designed and manufactured by Petit Pli Ltd.

Auxetic furniture has also attracted attention due to its functionality and design. A good way to describe this furniture would be to call it “furniture that you never get bored of” as you can change it as you want or need to. Imagine a table that can be made bigger by simply pulling it or shelves that can be adjusted depending on what you are trying to display (see Figure 10). Using *auxetic foams*, *i.e.* foams that have been transformed by pressure and heat treatment [the negative Poisson’s ratio may be explained by the incorporation of the rotating rigid units and/or the re-entrant mechanisms present at the microscale (see Figure 11)] in chairs may increase comfort by placing different foams in different positions, enhancing back support and improving posture, much needed in the digital age. The possibilities in this area are endless.



Figure 10. Shelves incorporating the rotating squares auxetic mechanism by Lee Sehoon.

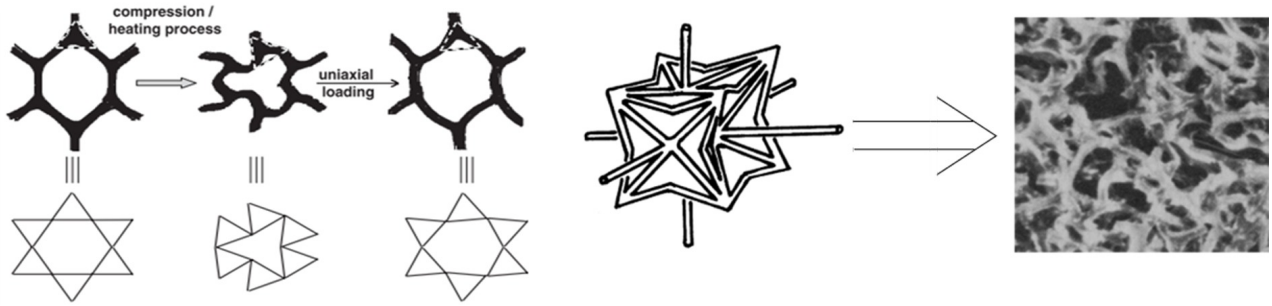


Figure 11. (Left) the rotating rigid-units explanation (Grima *et al.*, 2005) and (right) the re-entrant explanation (Lakes, 1987) for auxeticity in converted foams.

Another interesting application of auxetics is that of auxetic yarns, particularly those that also exhibit other enhanced properties such as high strength, lightness, high thermal resistivity and durability. Such high-tech yarns tend to have advanced applications such as protective gear for more extreme situations and military applications, such as ballistic protection. On the topic of ballistic protection, auxetics have found their way into a number of protective applications, which include, but are not exclusive to, military applications. Protection can be extended further from yarns, and research is being carried out on auxetic protective barriers, some of which have already been applied for ballistic protection as an alternative to yarns in order to reduce the shock wave of the blast due to vibration damping properties. Apart from the aforementioned ballistic protection, auxetic foams have also been suggested as a means to improve helmets for sports and motoring applications, and work is being carried out in order to determine the best distribution and foam to use. Similar propositions have been made for knee pads, shoulder pads and other protective equipment, and also on the incorporation of an auxetic hard shell on the outside of the protective foam in order to have a better fitting protective pad. A collage of protective applications of auxetics can be seen in Figure 12.

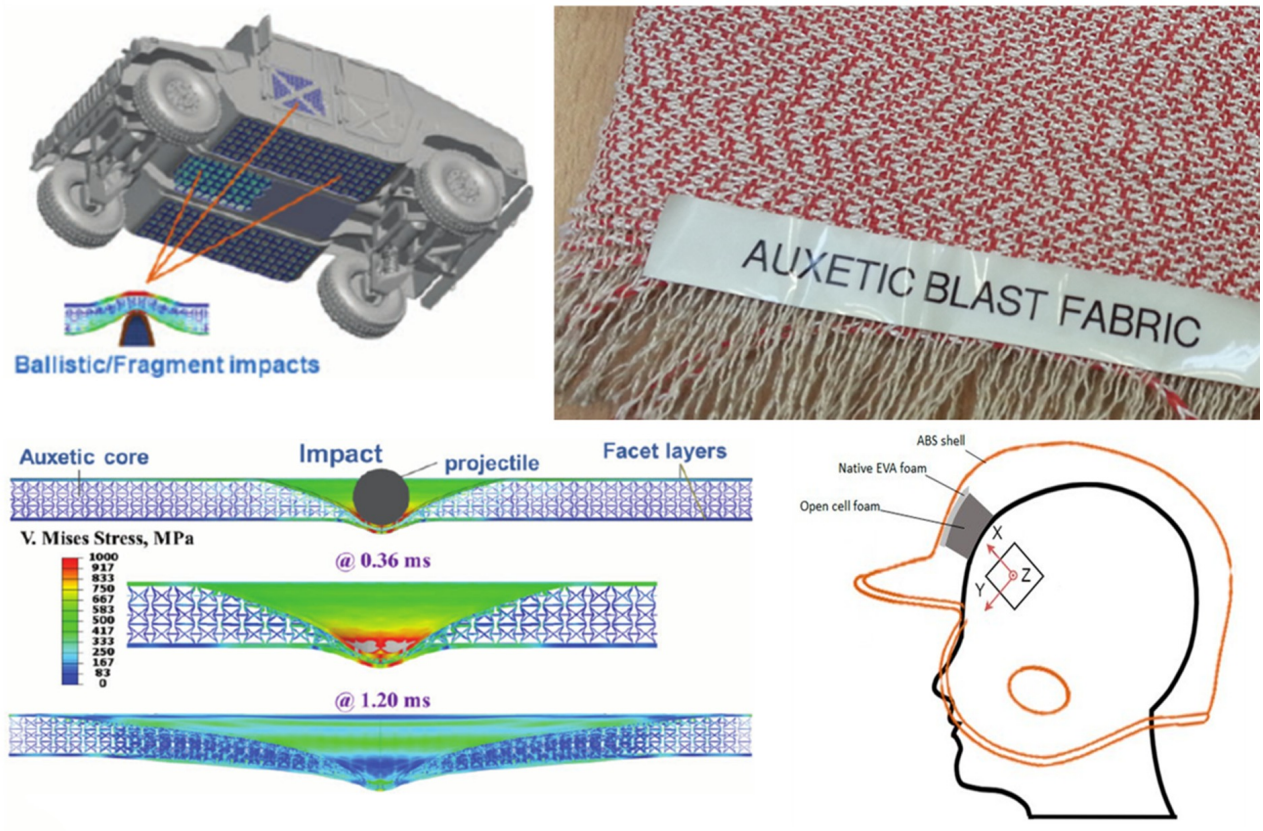


Figure 12. A collage of protective applications of auxetics, featuring (top left) ballistic protection applied to vehicles, (top right) blast protective fabric, (bottom left) blast protective glass curtain concepts and (bottom right) helmets incorporating auxetic foams.

Auxetic home-improvement applications have great potential as they simplify and improve such components. Examples include the auxetic nail, the auxetic screw and auxetic rivets, which become thinner when applying the component, making application easier, and become fatter when applying stress on the fully applied component, providing a better grip on the surface compared with the conventional counterparts. Similar applications of auxetics include seals and gaskets, which are expected to provide a better seal compared with non-auxetic components.

Going down further in size, in the boundary between macro- and microscale one can find auxetic stent applications. These small devices are designed to open up and keep open arteries that are blocked or have collapsed (see Figure 13). The stent itself has two important requirements: to be small upon entry to the circulatory system and to get longer and fatter when reaching its destination by means of a balloon-like device inflating it. These requirements fit perfectly into the applicability range of auxetic materials and structures, and therefore, auxetic stents are truly an ideal solution for this medical requirement.

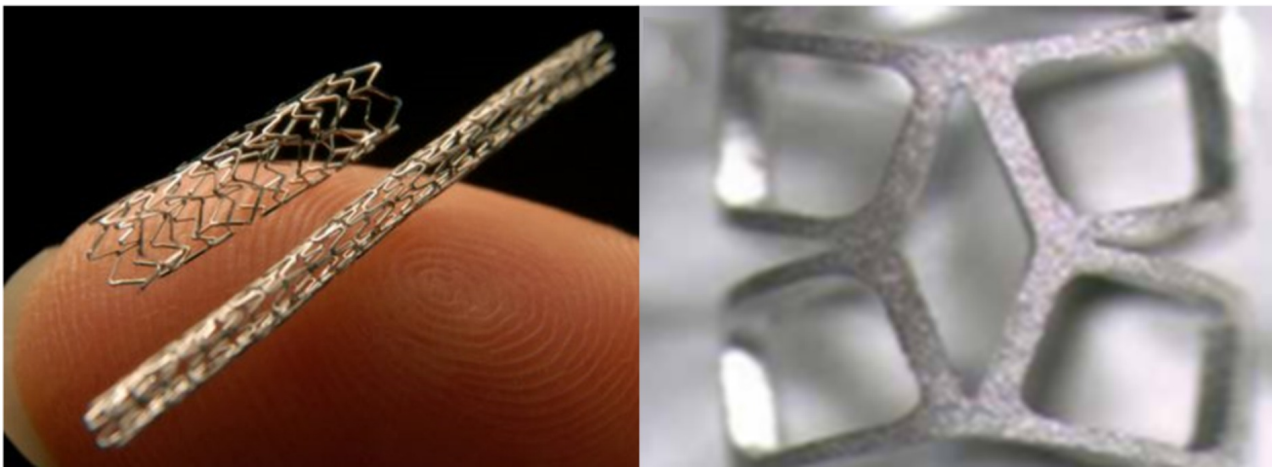


Figure 13. (Left) stents prior to application (iStock.com/RickLeePhoto), and (right) a section of an auxetic stent (Amin *et al.*, 2015).

Another possible medical application of auxetics is that of pharmaceutical-releasing dressings, a concept that was first proposed by A. Alderson. The idea here is that, for example, the pharmaceutical agent would be trapped within the auxetic pores (*e.g.* in between the rigid units in a rotating polygons model shown in Figure 14), and when the body part being treated begins to swell, as a result of the auxetic behaviour, the pharmaceutical agent will be released and the swelling/pain would be targeted at just the right time.

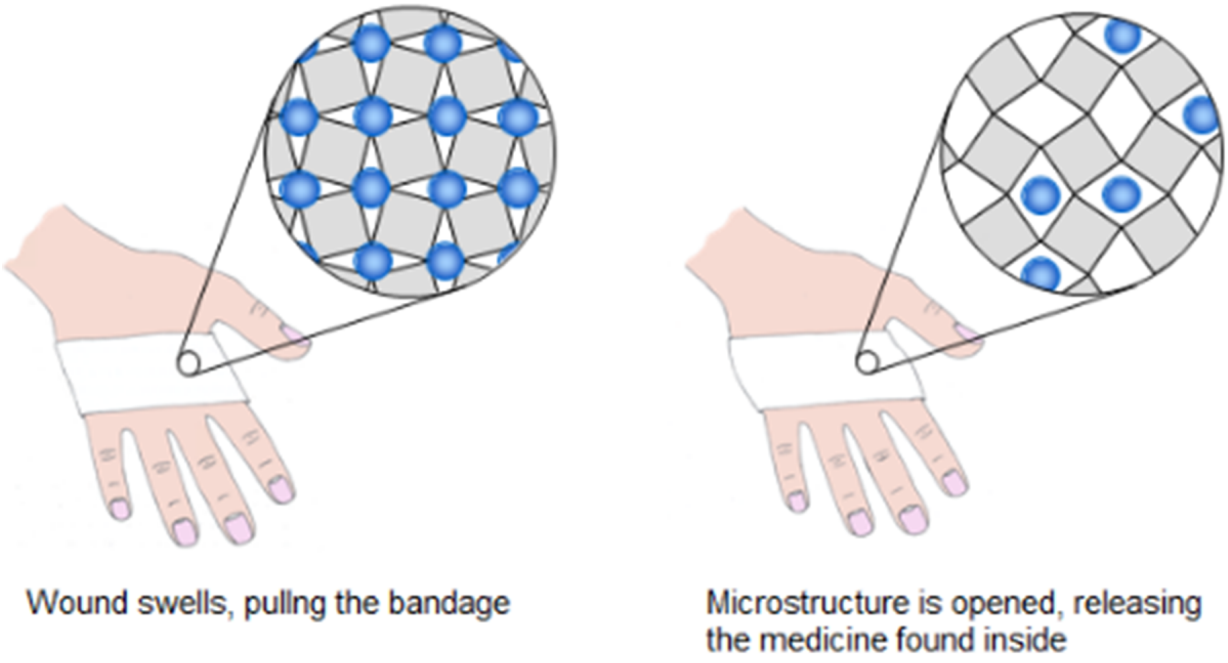


Figure 14. Auxetic smart dressings, which release the pharmaceutical agent when required.

Within the lowest scale to be discussed, the nanoscale, a possible application has been suggested for auxetic materials, namely nanofilters. Nanofiltration is filtration at the atomic/molecular level by means of filtration structures built of atomic networks. This is a suggested application of auxetic porous networks of the nanoscale, such as reflexyne, shown in Figure 15, having the ability to have their pore size changed in an auxetic fashion, *i.e.* the pores are size-tuneable by the application of stress.

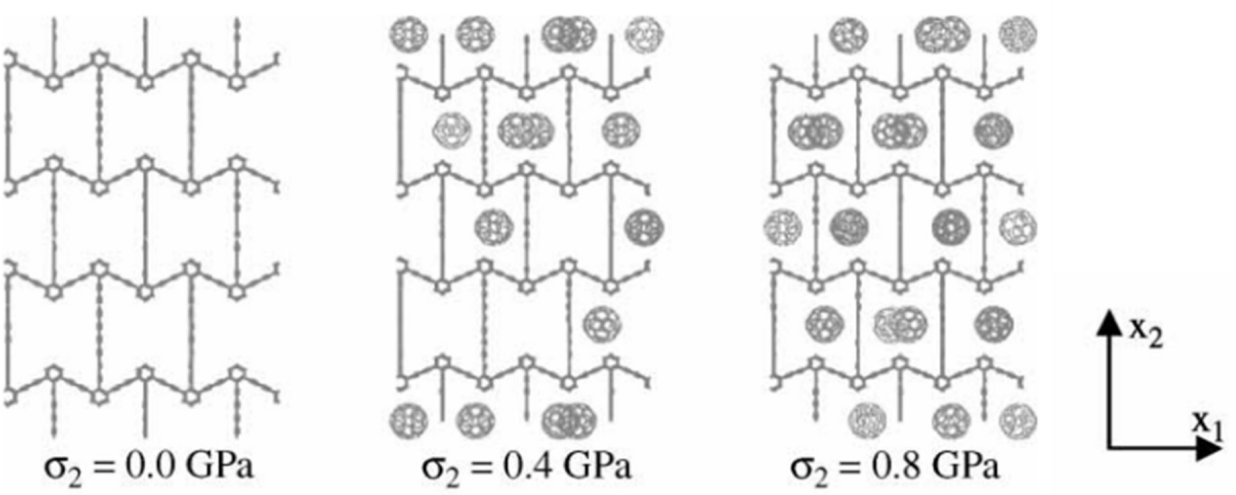


Figure 15. Auxetic reflexynes, which can be used as nanofilters (Alderson *et al.*, 2005).

Being a relatively new subject, it is certain that more applications will come about for this highly interesting mechanical property, and as the possible applications increase, so will the demand for materials that exhibit this remarkable property. This is expected to lead to further developments of novel mechanisms that generate auxetic behaviour, which in turn could once again result in other possible applications unknown to us as of yet. It is this continuous "chicken and egg" type research cycle that keeps auxetics driving in the fast lane … along with plain-and-simple curiosity.

I would like to thank Professor Mike Glazer for the opportunity to write in this Newsletter and for all his help in doing so.

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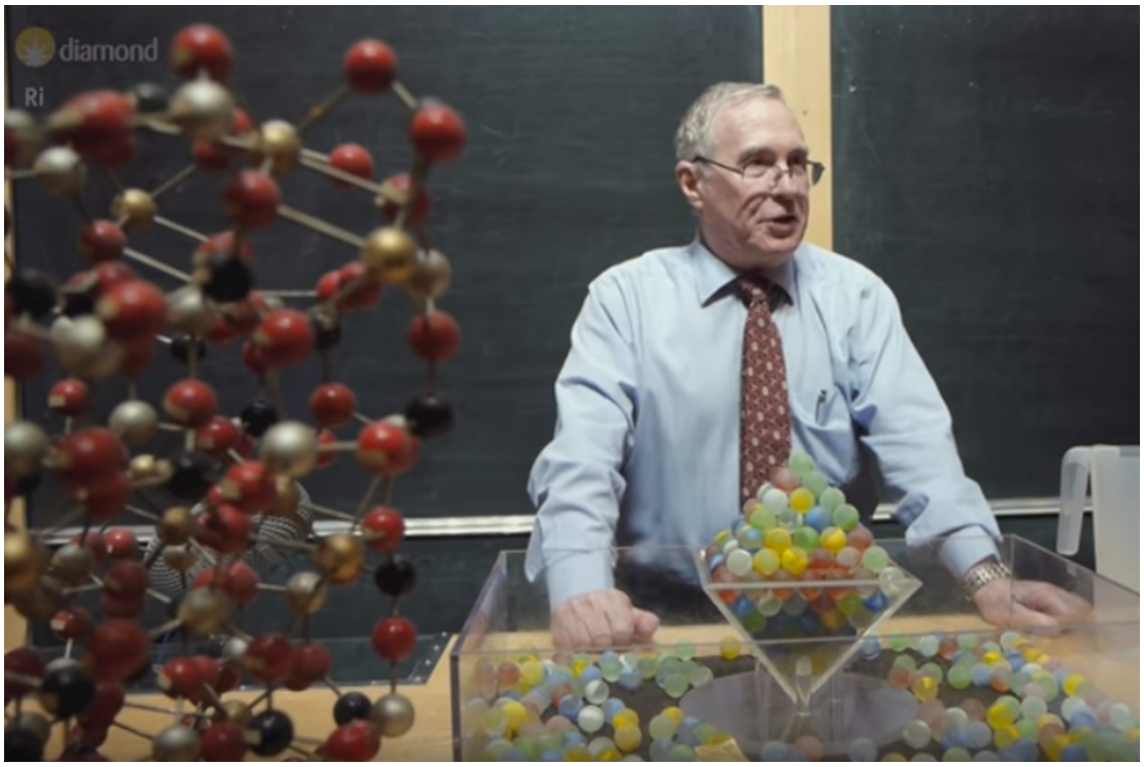
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Original article: https://www.iucr.org/news/newsletter/etc/articles?issue=142706&result_138339_result_page=9

FEATURE ARTICLE

Bragg's balls

Mike Glazer



It is well known that Lawrence Bragg was especially adept at presenting science to an audience in many ingenious ways and yet, at the same time, with great simplicity. In fact, he was particularly in his element when demonstrating to young people, saying “never talk about science, show it to them". I was fortunate enough to have been one of those teenagers who was able to attend his lectures at the Royal Institution in London, UK, and those occasions have stuck in my memory ever since.

When I moved from the Cavendish Laboratory, Cambridge, UK, to the Clarendon Laboratory, Oxford, UK, in 1976, I brought with me almost all of the crystallographic equipment plus many items of interest that dated from the days when Bragg had been the Cavendish Professor. These are now on exhibit in a small museum I set up some time ago in the Clarendon. In a previous issue of the *IUCr Newsletter*, I used one of the prototype boxes of Beevers-Lipson strips from my museum to explain how they were used (see https://www.iucr.org/news/newsletter/volume-26/number-1/how-did-they-do-that-beevers-lipson-strips).

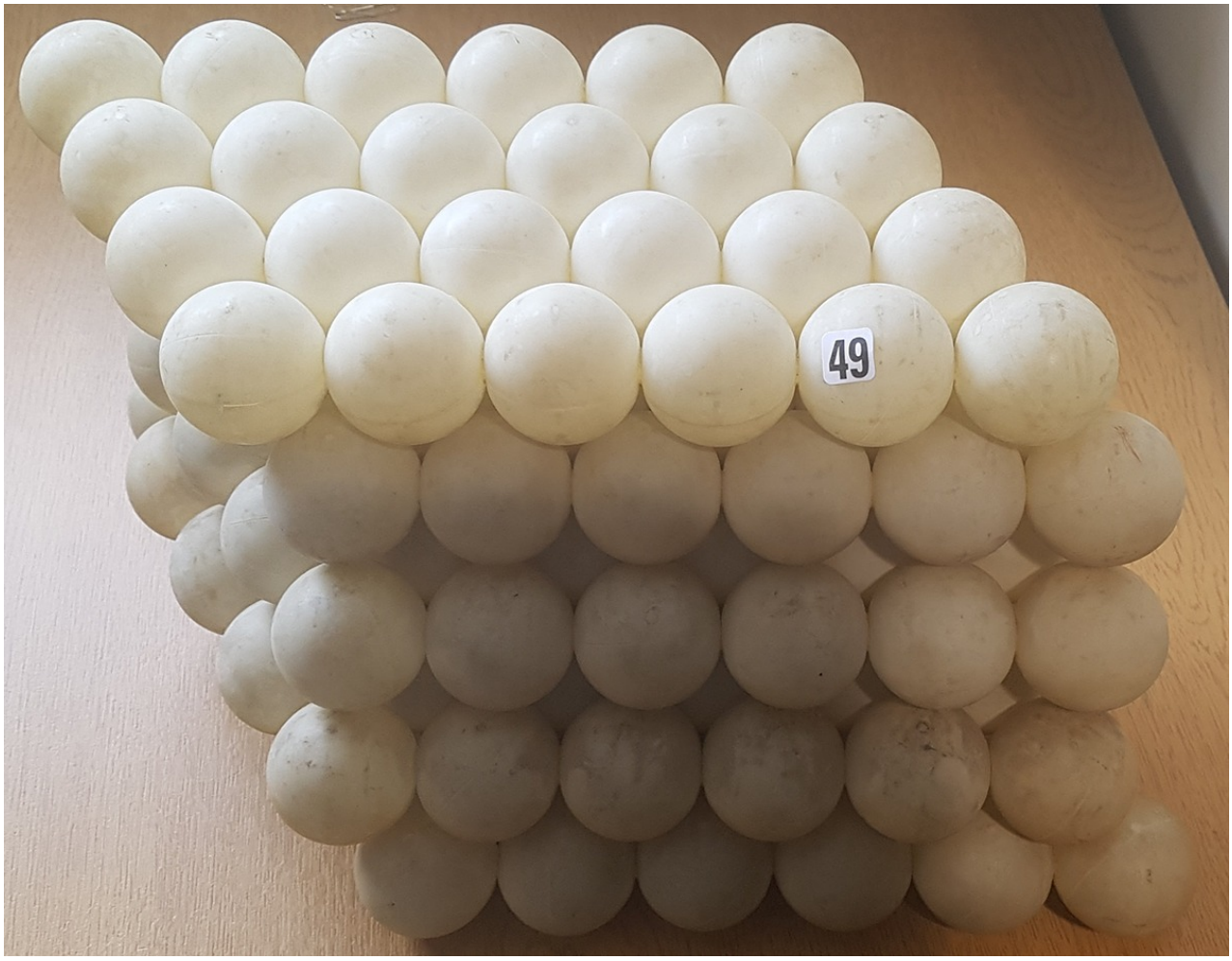


Figure 1. W. L. Bragg's ping-pong ball rafts.

Bragg was very keen on lecture demonstrations and, because he was clever with his hands, he made a number of items himself. In particular, he made use of ping-pong balls to illustrate how atoms pack together. Figure 1 shows one example from my museum: simple rafts of ping-pong balls to demonstrate how the structures of metals can be understood in terms of close-packing and how dislocations can form. You can see Bragg using this model in a video made in 1952 here and here.


Figure 2. Construction of an octahedron using four ping-pong ball layers.

Figure 2 is a nice variant in which four small rafts of ping-pong balls can be stacked together in the sequence ABCA to form a crystal in the shape of an octahedron. This simple demonstration is great for explaining to a student how cubic-close packing is created with this sequence and where to find the threefold and, more importantly, the locations of the fourfold (*i.e.* cube) axes.



Figure 3. W. L. Bragg's ping-pong model of the packing of naphthalene molecules.

In Figure 3 is a ping-pong model showing the crystal packing of molecules of naphthalene. Here Bragg has painted the balls black to represent carbon atoms. I recall being told by a technician at the Cavendish that this was one of Bragg’s favourite models. I am not sure when this was made but there is a photograph (Figure 4) of Bragg in Manchester in 1936 holding a model that looks suspiciously similar.

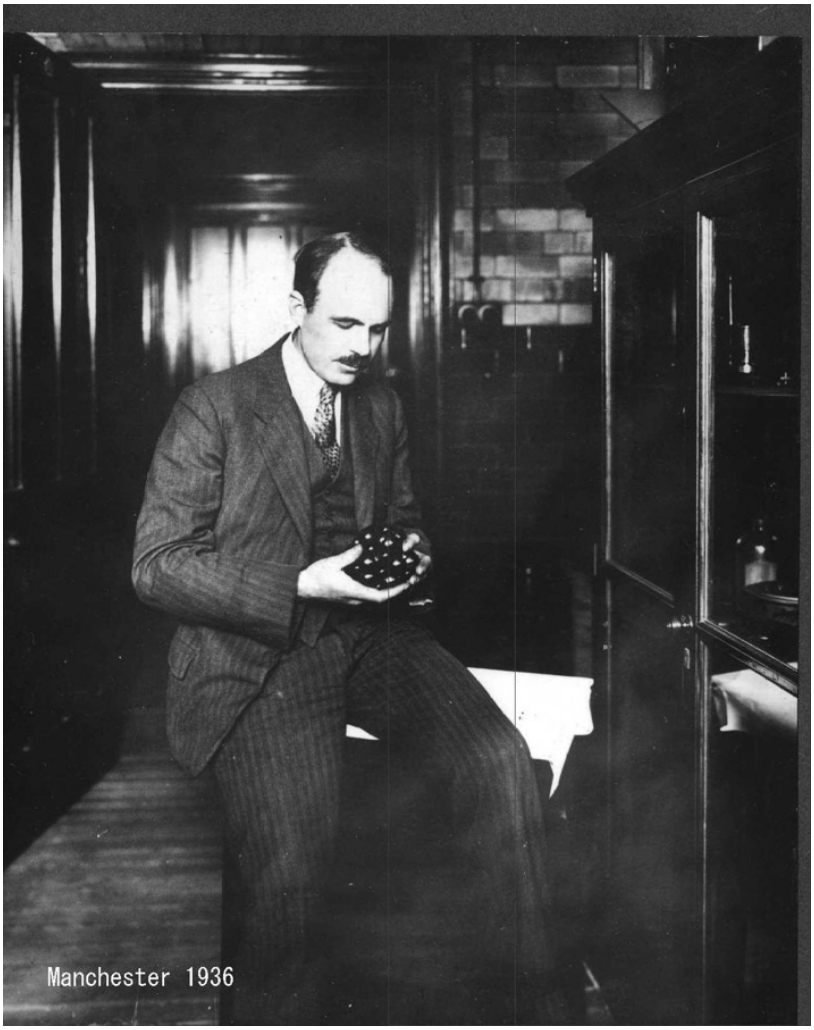


Figure 4. W. L. Bragg at Manchester University in 1936 (photograph from Robin Marshall).

Finally, there is an interesting demonstration of how crystals grow using marbles to represent atoms. This was filmed at the Royal Institution by the BBC in a series entitled *The Nature of Things*, presumably in the early 1960s (see here). Although the audience consisted primarily of adults, it was aimed at children and broadcast on children's television. Bragg, acknowledging the idea by John Desmond Bernal, starts with an ordered array of marbles contained within a plastic inverted pyramid acting as the bottom half of a crystal. He then pours more marbles on top and, as if by magic, the top half of the octahedron is formed. I remember being impressed with this demonstration and a few years ago I decided to reproduce the model.



Figure 5. Marbles demonstration: initial state.

Figure 5 shows my construction with marbles filling the semi-octahedron onto the (100) face. One thing that I noticed was that Bragg had to guide the flow of marbles somewhat with one hand, and I suspected that this was because his marbles were all shiny so that they tended to slip too much. However, I found that one can buy 22-mm frosted marbles. In order to determine the number to purchase, a useful formula for the number of spheres that can be packed into an octahedron (known as the octahedral number) is given by $O = n(2n^2 + 1)/3$, where n is the number of spheres along an edge. In my case I decided to have seven marbles on the edge, giving a total of 231 (expensive!). I added another 100 marbles (even more expensive!) to cater for any overspill. To construct the octahedral base, I cut four equilateral triangles of side 7 by 22 mm = 154 mm out of Perspex (Plexiglass) and glued them together (after chamfering the edges to make it look pretty). Four plastic support pillars were then glued at the bottom to enable the inverted pyramid to stand upright. I also constructed a large plastic surround box to collect all the spilt marbles. Figure 6 shows how this looks after pouring marbles randomly on top.

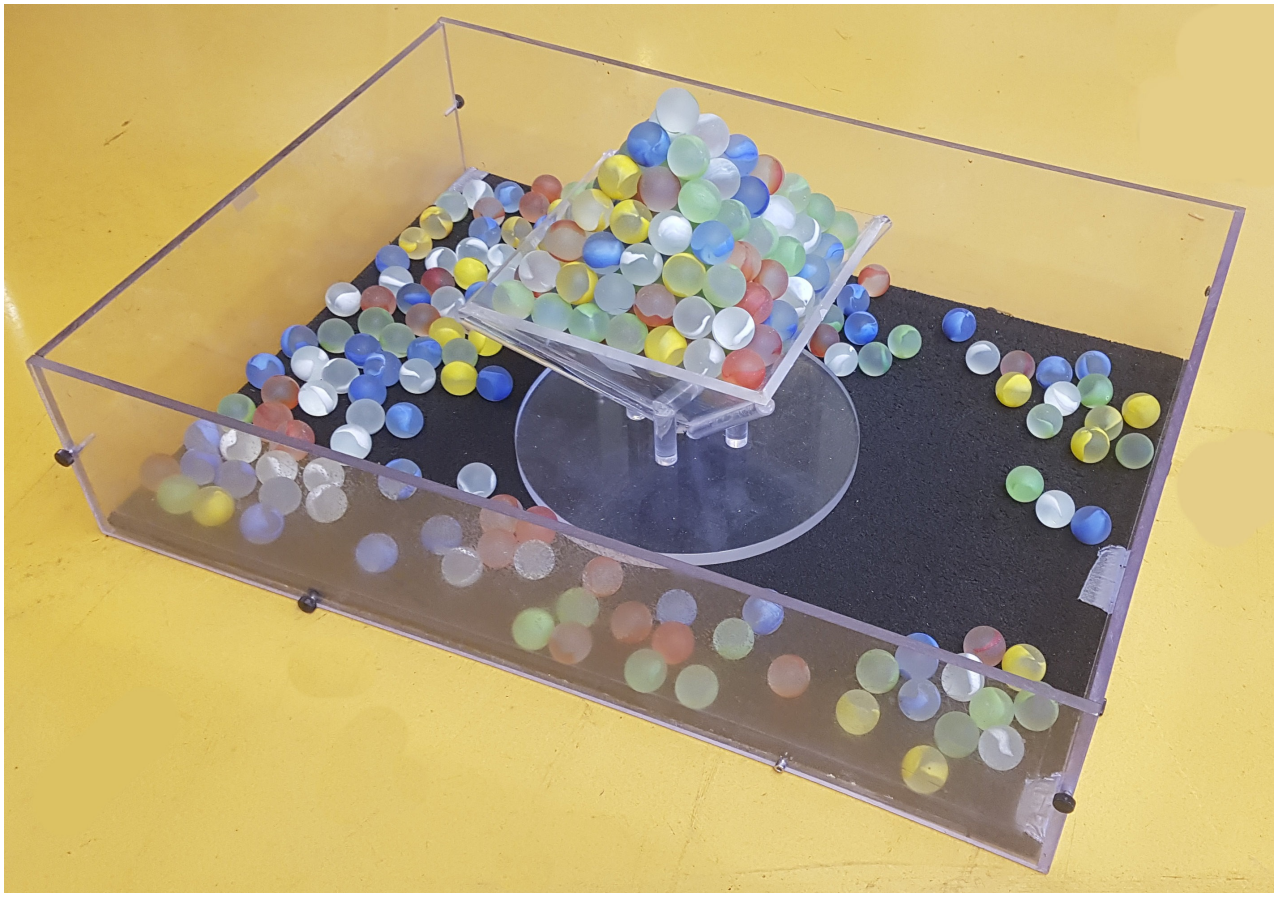


Figure 6. After pouring marbles on randomly to form a perfect octahedron.

You can see this in action in a film made during the 28th European Crystallography Meeting held at Warwick University, UK, in 2013, or in Figure 7 (with permission of Kathryn Boast, University of Oxford). Because the marbles are frosted, little guidance is now needed to get the top half of the octahedron to grow. I have used this demonstration with excellent success at schools and fairs. It is interesting to get the children to pour the marbles by themselves and then see their surprise at the result. For adults and older children, I usually start by asking them to guess what will happen when we pour the marbles on. Would the result be a random disorder, or an ordered arrangement? And what shape would be formed, if any? It is fascinating to see their expressions of wow! when they see what happens.



Figure 7. Extract from a video by Kathryn Boast (Oxford).

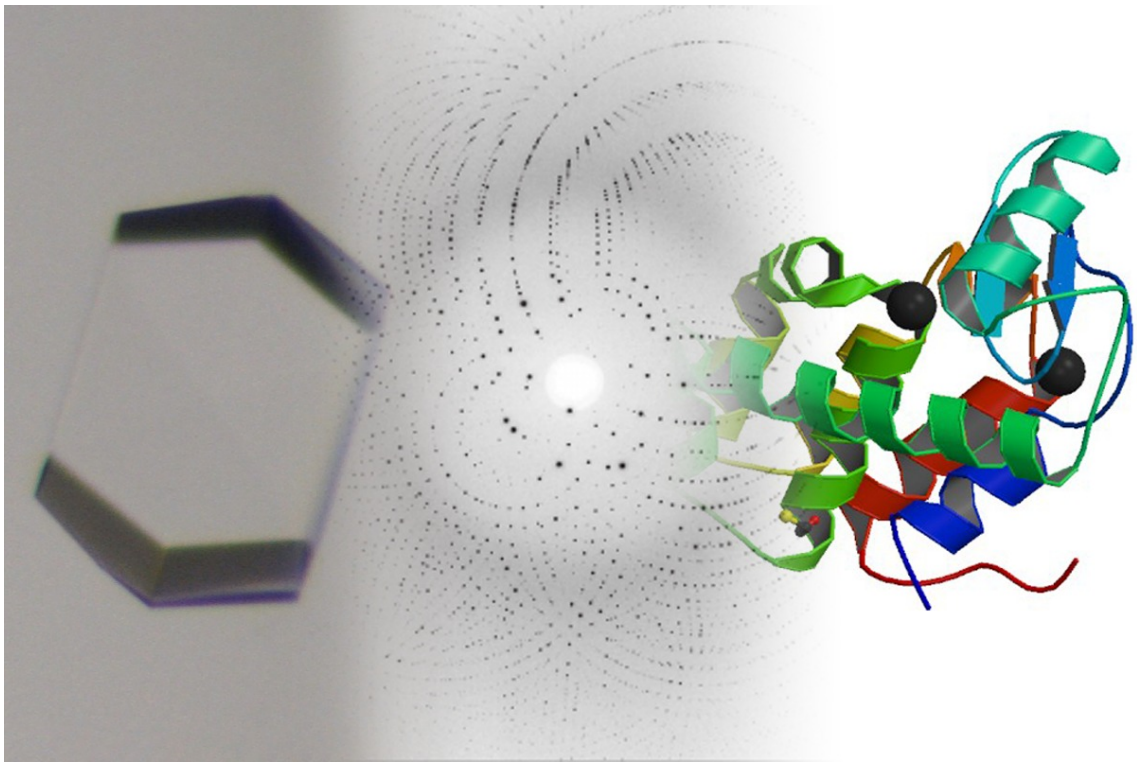
The reason that this works is interesting. First of all, gravity acts a bit like an attractive force holding the marbles (atoms) together and their physical size acts like a repulsion term. The first point to note is that if one starts with an ordered array, then there is a tendency to continue in an ordered fashion as each marble fits into the spaces between the marbles below. The magic formation of the octahedral {111} faces occurs because the density of packing of the spheres on these faces is approximately 15% higher than on the original (001) face. Atoms like to get as close together as possible to minimise their interaction energy by balancing attractive and repulsive forces. Have fun with this!

Original article: https://www.iucr.org/news/newsletter/etc/articles?issue=142706&result_138339_result_page=32

NOTICE

In numbers: initial screening at the MRC-LMB protein crystallization facility

Fabrice Gorrec



Crystallization is required for the determination of macromolecular structures with X-ray crystallography. Because the results of an initial crystallization screen using a particular macromolecular sample cannot be predicted, the approaches that lead to success can only be found empirically (Chruszcz *et al.*, 2008; McPherson, 2017). A very low yield of useful crystals from initial screening is to be expected for the vast majority of samples. The lack of sample stability or other sample problems, such as buffer incompatibilities, can render entire initial screens unsuitable for crystallization (Jancarik *et al.*, 2004). In addition to randomness inherent in the process, sample sensitivity to experimental fluctuations can also cause reproducibility issues during later optimizations.

One strategy to bypass some of these problems is to start with a large screen containing many different initial crystallization conditions. We have adopted such a strategy at the MRC Laboratory of Molecular Biology (MRC-LMB, Cambridge, UK), combined with an automated vapour-diffusion sitting drop technique for setting up crystallization droplets. To further simplify the process when dealing with large screens, crystallization plates pre-filled with reservoir solutions are made ready to be used (Stock *et al.*, 2005). Currently, our complete initial screen integrates 22 x 96-well plates = 2112 separate commercially available conditions (Gorrec & Löwe, 2018). Preparing the pre-filled plates and setting up the crystallization droplets represent the largest cost of our crystallization facility.

Here, I present some statistics collected over a decade of running the facility at MRC-LMB: the numbers of plates pre-filled with initial screening kits, the resulting costs and the final yields of quality diffraction crystals. We hope the data will be useful to those thinking about setting up a facility or for comparison purposes. The numbers also highlight a recent decline caused by the advent of a competing method that eliminates the need for crystallization – cryo-electron microscopy (cryo-EM) –, which now regularly produces atomic models comparable in quality to those obtained by X-ray crystallography (Nogales & Scheres, 2015; Henderson, 2018).

1. Production of pre-filled plates

Table 1 shows the number of plates pre-filled with initial screens that have been produced at the MRC-LMB over the last decade. The plates were produced by a fully automated and integrated system comprising a liquid handler (Tecan), a plate storage carousel (Tecan), an inkjet labelling printer (Markem-Imaje) and an adhesive plate sealer (Brandel) (Gorrec & Löwe, 2018). During a typical production run of the system, 72 MRC 96-well 2-drop crystallization plates (Swissci) are filled with a particular commercially available screening kit, and the process lasts around 4 hours. The system dispenses 80 µL of each reservoir solution, provided in 15 ml Falcon tubes, into the designated wells of the plate. After that, the pre-filled plates (referred to internally as 'LMB plates 1–22') are stored at 10 °C in incubators, where they are available to users.

Table 1. **Production of LMB plates. Note: while moving into our new building, operation of the facility was disrupted (2012–2013)**

Financial year	LMB plates
2009–2010	7500
2010–2011	7599
2011–2012	7562
2012–2013	3867
2013–2014	6357
2014–2015	6985
2015–2016	6825
2016–2017	4450
2017–2018	3539
2018–2019	4388
TOTAL	**59,072**

In recent years, it can be observed that the number of LMB plates produced has decreased from a peak in 2014–2015. The main explanation is the success of cryo-EM, which has meant that many projects have shifted to this revolutionary method of structure determination at near-atomic resolution. Furthermore, at MRC-LMB, we see that for larger

proteins and complexes, X-ray diffraction has almost exclusively become a supporting technique to cryo-EM when high-resolution structures of particular protein domains of interest or detailed chemistry need to be investigated. This often requires the elemental contrast offered by X-rays and anomalous scattering methods for which cryo-EM has currently no workable equivalents. In contrast, fragment screening and high-throughput structure determination of small molecule–protein complexes has remained the domain of X-ray crystallography, mostly because of the differences in resolution attainable routinely by the two methods and the speed achievable with crystallography once phases are available.

2. Costs

Table 2 lists the costs for consumables when setting-up droplets in an LMB plate with a stand-alone Mosquito nanoliter dispensing robot (TTP Labtech). We found that in most cases, our users set up single droplets per experiment (*i.e.* 96 droplets per plate), which is often required to preserve sample freshness. This also avoids the chance of carry-over and confusion around sample identity. We have calculated that the cost for consumables is close to GBP 15.00 per LMB plate (USD 20.00), including pre-filling and drop setting. This multiplies to GBP 330.00 (USD 432.00) for a complete initial screen using all 22 LMB plates. All calculations exclude the initial and running costs of liquid-handling equipment and labour.

Table 2. Consumable costs for setting up a 96-condition initial screen in LMB plates at the MRC-LMB

Item	Cost GBP (USD)
Plate	5.96 (7.79)
Screen (avg.)	5.48 (7.16)
Tips	3.61 (4.72)
Seal (est.)	0.03 (0.04)
TOTAL	**15.08 (19.71)**

With a high turnover, robust equipment (*i.e*. with a life span of 10 years or more), in-house maintenance support and thorough optimization of the automated protocols, the costs related to equipment have been reduced significantly. We have estimated this cost to be an additional GBP 5.00 (USD 6.50) per plate at MRC-LMB. This means an overall cost of GBP 20.00 (USD 26.00) per plate excluding labour. The full production of initial screens during the financial year 2018–2019 was hence 20 x 4388 plates = GBP 87,760 (USD 115,000). This might seem a lot but should be considered in the context of projects where crystallization decides between success and failure, when so many variations of samples must be tried. It would be interesting to put this in relation to the current costs of cryo-EM structure determination, mostly caused by costly equipment and its maintenance, and expensive consumables such as grids, rings and cartridges.

Our protocols to set up crystallization droplets in a 96-well crystallization plate are relatively fast, lasting 5 min overall in most cases. In fact, the most time-consuming task is the subsequent assessment of the experiments by microscopy. There are commercially available automated imaging systems that can help with imaging and assessing the experiments, but we decided against such infrastructure. Our level of throughput would require an imager with a very large plate storage capacity and fast image processing, which would represent a very significant additional cost component. In addition, practically, we found that investigating the results through a manual high-powered and high-quality stereo microscope is still the best possible way and ensures that hopefully no crystals are missed, however small and hidden they are within the droplets.

3. Yield

There is no laboratory information management system (LIMS) implemented at the MRC-LMB that would enable us to collect overall statistics. We found that this can slow down progress of each user because of the additional reporting burden. For example, a crystal hit might turn out to be useless later and this information needs to be tracked (only to erase it and make overall statistics more relevant). We have hence compiled a basic web-based data mining tool instead, which essentially generates details of conditions selected by users (who will handle their records independently).

Table 3 shows examples of results from our initial screening against various samples for which useful crystals could be obtained (the degree of sample optimization rounds varied from a few to 50 constructs/variants) (Gorrec, 2015). According to this subset of data, despite our large screen size, the yield of useful crystals is below 1%. In fact, a relatively high proportion of initial screens fails to produce useful crystals, while in a relatively low number of cases, a high yield is observed. Overall statistics would hence show a (much) lower yield than what is calculated from Table 3. This might not seem to be encouraging but, again, it needs to be considered in the context of users who attempt crystallization with a broad variety of novel samples. Besides, this should be put in relation to yielding useful data from cryo-EM screening for suitable imaging conditions, which in our experience can also be frustratingly low.

Table 3. **A short list of example results from users' initial screening against various samples where useful crystals were obtained. According to this subset of data, the average yield is 13/1466 x 100 = 0.89%**

Sample name	MW (kDa)	Conditions	Hits
Prp8	220	1536	2
HIV-capsid domain	36	1632	20
SUN	25	1632	80
Hexameric HIV-1 capsid	144	1632	30
Spliceosomal RNA helicase	240	1632	2
Mex67:Mtr2	73	1632	1

Sample name	MW (kDa)	Conditions	Hits
Atg13	32	1728	2
Arl1-BIG1(DCB domain)	50	1824	6
Cmd1	16	1440	2
MMK	38	1440	3
AVERAGE	**79**	**1466**	**13**

Based on the set of chemicals used to formulate the conditions that have been employed in earlier times (2002–2009, initial screen = 1152–1440 conditions) and the resulting published structures, it has been shown that suitable reagents and their nature/concentrations making up the conditions have virtually all the same importance in the process of structure determination (Gorrec, 2015). To us, this means that starting with the largest possible screen (given effort, cost, sample availability *etc*.) is to be encouraged and it has also motivated the development of further initial screen conditions (Gorrec & Zinzalla, 2018). Finally, it also means that further developments, such as the reduction in sample consumption (Wu *et al*., 2015), could still make a big difference in the overall success of our strategy.

The whole initial screening process at the MRC-LMB can be viewed at https://www.youtube.com/watch?v=iWbFkZUZOko

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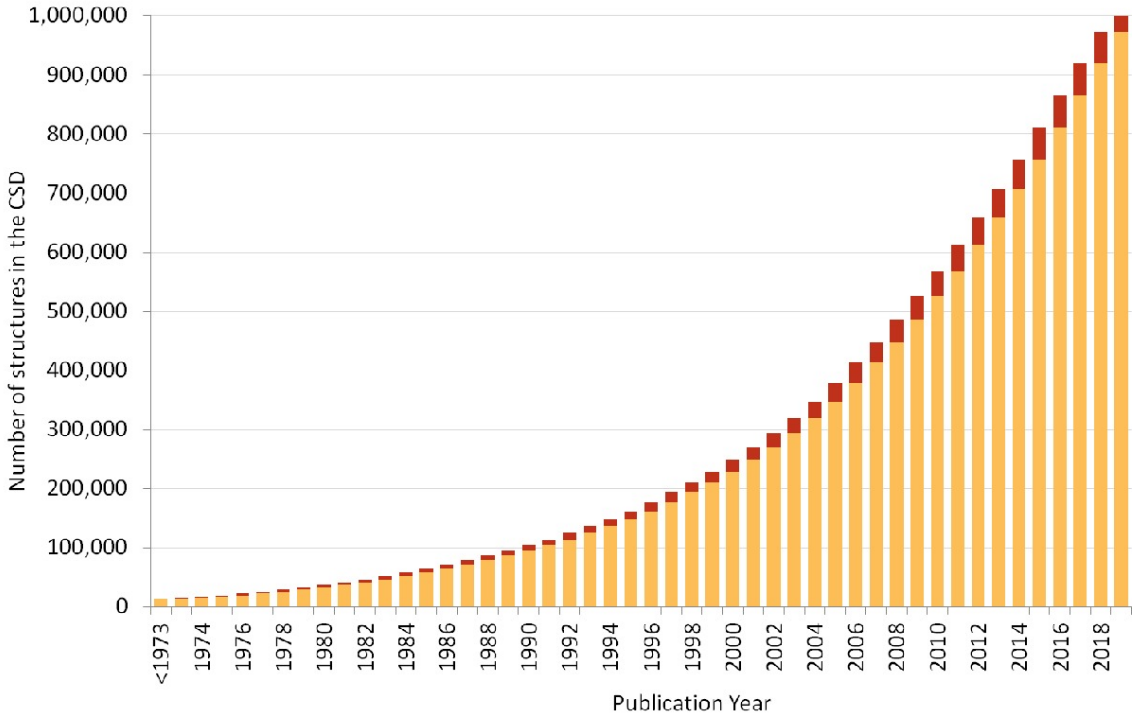
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NOTICE

Big data leads the way for structural chemistry



Growth of the CSD since 1972. The red bar shows structures added annually. Date: 6 June 2019.

On 6 June 2019, the Cambridge Crystallographic Data Centre (CCDC) announced a huge milestone for structural chemistry with the addition of the millionth structure into the Cambridge Structural Database (CSD).

The CSD is the world's repository of highly curated experimentally determined organic and metal–organic crystal structures. It is used globally by scientists in over 70 countries to understand how molecules behave and interact in three dimensions in the solid form and ultimately how this affects physical properties.

As the interest in ‘Big Data’ continues to grow in a time where machine learning and automation are changing the way pharmaceutical, agrochemical and many other industries work, reaching such a significant milestone is a huge achievement for the CCDC and the wider scientific community that contribute to and rely on this resource.

Large volumes of data such as this enable scientists to generate more replete answers from a more complete and diverse volume of information, ensuring confidence in the insights being drawn from the data. Furthermore, CCDC’s focus on ensuring the integrity of the data within the CSD through stringent quality assurance and control steps adds even more value and confidence that scientists are obtaining the highest quality information to inform their research.

This rich data resource, alongside advanced search, 3D data mining, analysis and visualisation software from CCDC, enables scientists from both industry and academia to further their research and predict new outcomes. In addition, knowledge derived from the CSD underpins computational chemistry and molecular modelling and is relied on by industry for the development and manufacturing of new drugs and within academia to teach chemistry.

Jürgen Harter, CEO of CCDC, commented ‘This is truly an important milestone not only for CCDC but also for the wider scientific community. In addition to the value that lies in large sets of data like this to help scientists inform their research and decision making, we also pride ourselves on the high quality of the data, a result of the hard work of our expert in-house database team. Maintaining a policy of strict data interrogation ensures the value of the plentiful insights that can be drawn from the CSD, avoiding misinformation that can lead to wasted time, resources and ultimately cost.’

The 1,000,000th structure is an *N*-heterocycle produced by a chalcogen-bonding catalyst activating multiple reactions steps sequentially. In the paper the authors describe a class of extraordinary chalcogen-bonding catalysts that enable the assembly of discrete small molecules leading to the construction of *N*-heterocycles in a highly efficient manner. The structure was determined by Yao Wang and co-authors from Shandong University in China and published in the *Journal of the American Chemical Society* (JACS).

‘We’d like to congratulate Yao Wang and all of his co-authors, for publishing the millionth structure and we are so grateful to the 350,000 plus scientists from around the world that have contributed their data, enabling us to reach this milestone and placing the CSD as the go-to resource for structural information within the scientific community’, said Suzanna Ward, Head of the CSD.

Dr Wang commented ‘We are delighted to hear that our structure [1-(7,9-diacetyl-11-methyl-6*H*-azepino[1,2-*a*]indol-6-yl)propan-2-one; CSD Refcode XOPCAJ] is the millionth structure to enter the CSD! We have used the CSD for over 10 years because it is an excellent platform to report new crystal structures and an outstanding database to find inspiring chemical structures. It is a valuable resource to us and to many other scientists around the world so we are very proud to be associated with this milestone for the community.’

Peter Stang, Editor-in-Chief, JACS, said 'We are delighted to hear that the millionth structure in the CSD was published in JACS. We know our readers value the CSD as a trusted repository of structural data and some of our authors have demonstrated how this rich resource can accelerate scientific research. Our continued collaboration with the CCDC helps make this wealth of data more accessible to the community as well as helping us ensure the integrity of data published in our journals and we are proud to be associated with such a significant milestone in structural chemistry.'

When asked what’s next for the CSD, Dr Harter commented that although the use of the CSD in the pharmaceutical and agrochemical industries is already well-established, it is now fast becoming a fundamental resource for research into new materials such as batteries, paints, pigments and dyes, and in particular the development of gas storage

frameworks and tailored catalysts. As environmental contamination and sustainability become increasingly important there is considerable potential on a global scale.

CCDC has noted a consistent rise in deposits from research taking place in China over recent years. 'It is an exciting time for life science and materials development research with markets such as China leading the way in scientific discovery. We are excited to see what insights we obtain from this market going forward,' Dr Harter commented.

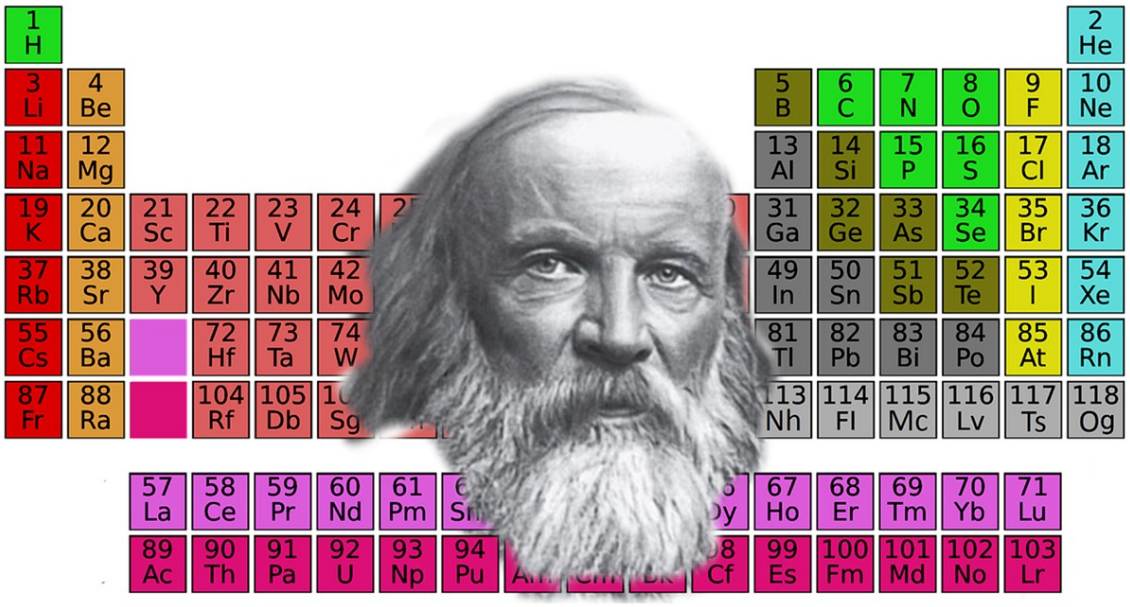
CCDC also has plans to further draw on insights and trends from the data to inform the direction of future research across different industries.

This report is taken from a press release issued by the CCDC. For more information, see here or contact Lucy White. See also Suzanna Ward's article in this issue of the IUCr Newsletter.

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NOTICE

Materials Union endorses UNESCO's IYPT2019



The seminal work of Dmitri Mendeleev 150 years ago revealed systematic interrelationships of all the chemical elements known and predicted at the time and, remarkably, of those subsequently discovered. Those elements are the stuff of which everything and everyone we see is made. The phenomenal natural evolution of our world, including of life itself, assembles the necessary major and often crucial minor elemental ingredients required for Nature's grand design. Mendeleev's Periodic Table of the Chemical Elements and its legacy gave us the tools and understanding to invent and design well beyond what Nature has provided.

Whereas empirical uses of materials date to the Bronze and Iron Ages, our electronics, pharmaceuticals and skyscrapers owe their existence to invention informed by knowledge of the properties of the elements and of the likely properties of myriad compounds and alloys that they form. Such research and invention continue apace in the laboratories of universities and companies with no end in sight. The community of materials researchers depends on, and fully participates in, this exciting progress. The International Union of Materials Research Societies (IUMRS) therefore enthusiastically endorses UNESCO's declaration of 2019 as the International Year of the Periodic Table of Chemical Elements (IYPT2019).

According to IUMRS President Y. F. Han, "The thousands of researchers affiliated with our membership, who devote their careers to uncovering the next great innovation enabled by advanced materials, all rely on their early training which included Mendeleev's Table and

which remains invaluable in formulating the next new approach to solving problems and making new discoveries in the laboratory. It is therefore entirely appropriate for IUMRS to recognise this sesquicentennial anniversary on their behalf."

The IUMRS is an association of some 14 professional societies spanning Asia, Africa, the Americas and Europe. Member societies serve scientists, engineers and sponsors who perform and support research on advanced materials and devices for the betterment of humanity and the planet. The IUMRS, which is a member of the International Science Council, has offices in Beijing, China; Singapore; Strasbourg, France; and Evanston, IL, USA.

This report is taken from a press release issued by the IUMRS. For more information, contact Fenfen Liang, Director, IUMRS Head Office.

The IUCr is a sponsor of IYPT2019.

Original article: https://www.iucr.org/news/newsletter/etc/articles?issue=142706&result_138339_result_page=18

The IUCr’s good works aka why you should send your best articles to IUCr journals

Alex T. Ashcroft



IUCr Executive Secretary, Dr Alex Ashcroft (execsec@iucr.org).

By the time this issue of the *Newsletter* is published, it will be two years since I joined the IUCr. When I was preparing for my interview for the position of Executive Secretary, I read the Triennial Report from the Montreal Congress and was hugely impressed by the generosity of spirit of the IUCr members and the sense of a crystallographic community. Whether it was editors donating their hard-earned honoraria to the Education and Outreach Fund, Commission members giving their time to organise schools and workshops or the IUCr itself providing money it couldn’t afford to support scientific meetings, it was clear that this was an organisation and a community that really cared, and that believed in the value of what it was doing. After more than 20 years working for a large multi-national company, it was very refreshing and extremely motivating to read.

Two years on, those things still impress and motivate me, but I have been surprised that much of the IUCr’s light seems to be hidden under the proverbial bushel, particularly at a time when the IUCr is fighting to survive in a very difficult economic environment, so when Mike Glazer asked me to write something for the *Newsletter*, I was delighted to take this opportunity to let people know what we are doing, and why we would love you to think of the IUCr journals when you are deciding where to publish your best papers. In the last issue, Massimo Nespolo warned you about unscrupulous publishers; now I can tell you why the IUCr is different.

Those of you who have looked at the IUCr's accounts at the ends of the Annual Reports in *Acta Cryst. A* will have noticed that the IUCr lost about USD 2 million between 2013 and 2016. A few more years like those, and the IUCr would have emulated John Cleese's parrot and "ceased to be". Even with the cost-cutting measures that the Finance Committee has implemented, we still only recorded a surplus of around USD 20,000 for 2018. Despite this, from the Executive Committee to the Finance Committee to the Sub-committee on the Union Calendar, the determination to continue to support young scientists, Education and Outreach and the Africa initiative is very apparent. Since 2014, the IUCr has spent over USD 1.6 million on these causes, and probably the most rewarding part of my job is to be able to distribute financial support to schools and workshops around the world. Apart from the IUCr's accounts, the Annual Reports also list the meetings that the IUCr supported that year (usually in section 7), and you can also find them on the IUCr's website here.

Apart from supporting the meetings themselves, we also offer IUCr books and open-access vouchers to IUCr Journals poster prize winners. Another uplifting part of my job is when I hear from an editor, author or Commission member that early in their crystallographic career they were the recipient of an IUCr award and that the service they are now providing to our community is to help to pass that opportunity on to another generation.

The IUCr accounts also show that almost all of the IUCr's income comes from its journals. The hard work and dedication of the Editors, Co-editors and Chester staff are vital to this, but we don't forget the important contributions of the reviewers and the authors. We know you have a choice of where to publish your papers, and we are grateful to those of you who choose to publish with us. We haven't outsourced any of our publishing operation, so your papers receive the personal attention of one or more members of our Chester staff and if you haven't published with us before, you might enjoy the experience of working with staff who care as much about your paper as you do. You can also take pride in the fact that your paper is helping to support our journals, and that the income from our journals is supporting our Outreach and Education efforts around the world.

An important part of the IUCr that I haven't yet mentioned is the IUCr's scientific Commissions and Committees. You can read about their hard work in the Annual Reports (usually in section 6). If we are going to survive, it's important that our Commissions and our journals support each other, so the Executive Committee has encouraged each Commission to publish a review or lead article in an IUCr journal during the triennium, and the journal editors are keen to hear from the Commissions as to how they can better serve their needs.

Finally, if you would like to support the work of the IUCr, you could join our Associates Programme. Of the benefits we offer to Associates, the 50% discount for personal use copies of *International Tables* seems to be the most popular. I haven't needed to use any of my Associate benefits, but every time I put on the lapel badge, I'm reminded of how I felt when I read the Montreal report, and I'm grateful for the opportunity to have joined this great community.

Original article: https://www.iucr.org/news/newsletter/etc/articles?issue=142706&result_138339_result_page=11

IUCR CONGRESS

IUCr2020: Workshop and meeting of the International Programme Committee

Radomír KuželIvana Kutá Smatanová



Radomír Kužel (Congress Chair, left) and John Helliwell (CommDat Chair and Commission on Crystallographic Nomenclature Member) enjoy a break after the first day of the IPC meeting.

It is a tradition of IUCr Congresses that the programme is put together during a three-day meeting of the International Programme Committee (IPC), usually in a location close to the Congress venue. When we discovered in Hyderabad at the last IUCr Congress that the costs for future IPC meetings would not be covered by the IUCr budget, we considered cancelling such a meeting and discussing everything online. However, our own experience and the advice of preceding organisers of IUCr Congresses led us to the conclusion that the IPC meeting should still go ahead and that we would find a way to organise it. Such a face-to-face meeting can be very efficient in comparison with sometimes endless email discussions.

During discussions on the form of the meeting, we took into account that this will be the 25th anniversary of the Congress and therefore it would be worthwhile to prepare some overviews about what is going on in crystallography. As the scientific work of the IUCr is conducted through its Commissions, we asked them for their help. We suggested that, in addition to the IPC meeting, we could start with presentations from all the IUCr Commissions (*i.e.* their representatives in the IPC) in a one-day event, which we called the *Current Trends and Future of Crystallography* (CTFC) workshop, and open it to the

public. We also made an effort from an early stage to communicate quite frequently by email with Commission and IPC members in order to keep their discussions on the Congress alive and avoid just picking up the topics a few hours before the deadline. It appeared that everything was useful and well accepted and led to very efficient work by the IPC. Therefore, we can recommend it for future Congresses, and summarise the basic points below.

Early setup of the IPC

As early as the 24th IUCr Congress in August 2017, the Commission Chairs were asked to select their representatives for the Prague Congress IPC. In December 2017, the Commissions were asked to submit more candidates for consideration. Having extra candidates is useful and also necessary to have a chance of creating an IPC with a good gender and regional balance.

In spring 2018, we selected the IPC members and sent out emails, inviting them to accept the role and providing a list of tasks. The IUCr Executive Committee approved the IPC in May 2018.

Then the place and time of the IPC meeting and CTFC workshop were determined. From dates offered during March to May 2019, only one week in May seemed to suit everyone. Announcing the date early is useful for the committee members as they can plan well ahead and may be able to take advantage of better hotel and travel prices.



IPC members and guests in the Prague Congress Centre.

IUCr Commissions

In August 2018, all IUCr Commission Chairs were sent a request to prepare a text for presentation by their IPC representative at the CTFC workshop; each speaker slot would be approximately 15 minutes. This initial request was followed by several reminders with deadline extensions from 1 March 2019 to the end of April 2019. The instructions for the texts were as follows:

'As the IUCr Commissions are different we are not imposing any strict restrictions on the text length or the content. All contributions should start with a short description and

explanation of the Commission subject. This can be followed by more detail if there are more streams in the subject, examples of advances achieved, highlights from previous years, problems to be solved *etc*. The activities of the Commission can be mentioned, in particular in connection with the above items, but they should not be the only element.'

Database-driven software for online input, editing and lists of everything

A true online database allows for very flexible work and the easy generation of different lists, categories *etc*. Our database was designed and prepared in autumn 2018 but the scripts are being modified continually. The IPC members have had access to the data from the beginning and, of course, most importantly, during the IPC meeting. In addition to the lists ordered by Commission, priority and, for people, region, country and gender, the so-called classified lists were generated according to the fields of interest in a similar way to the ECA focus areas. They were also used to create some balance between these areas in the programme. Unlike the ECA, multiple assignments of the lectures and sessions were allowed. The classifications used were Biological and macromolecular crystallography; Physics and fundamental crystallography; Materials and minerals; Chemical crystallography, structures; Methods, instrumentation; Theory, computation, modelling, data, standards; and General interest.

CTFC workshop

This full-day workshop was organised at the Prague Congress Centre on 14 May 2019. After a short opening, an introductory speech on current trends and the future of crystallography was given by one of the sponsors – Dubravka Sisak-Jung from Dectris – and then each Commission representative gave a short presentation. The proceedings have been published in *Materials Structure*.

In addition to the IPC members, the workshop was open to other participants giving a total number of 70 people. After lunch, the participants had a chance to see the whole Congress Centre in an hour-long excursion. The programme ended with dinner, and a few of us also attended the evening concert by Toto Cutugno, which was held in the hall where the Congress Opening Ceremony and plenary lectures will take place.

This was the first time such a meeting had been organised but we think that it was well received, and some of the IPC members strongly recommend that it should be repeated in advance of future Congresses. It is especially helpful that all the IPC members can see from the beginning the problems and topics of all the other Commissions. The subsequent discussions about the programme are then easier and compromises can be much better achieved.



The IPC admires the magnificent view from the Prague Congress Centre during their excursion.

IPC meeting

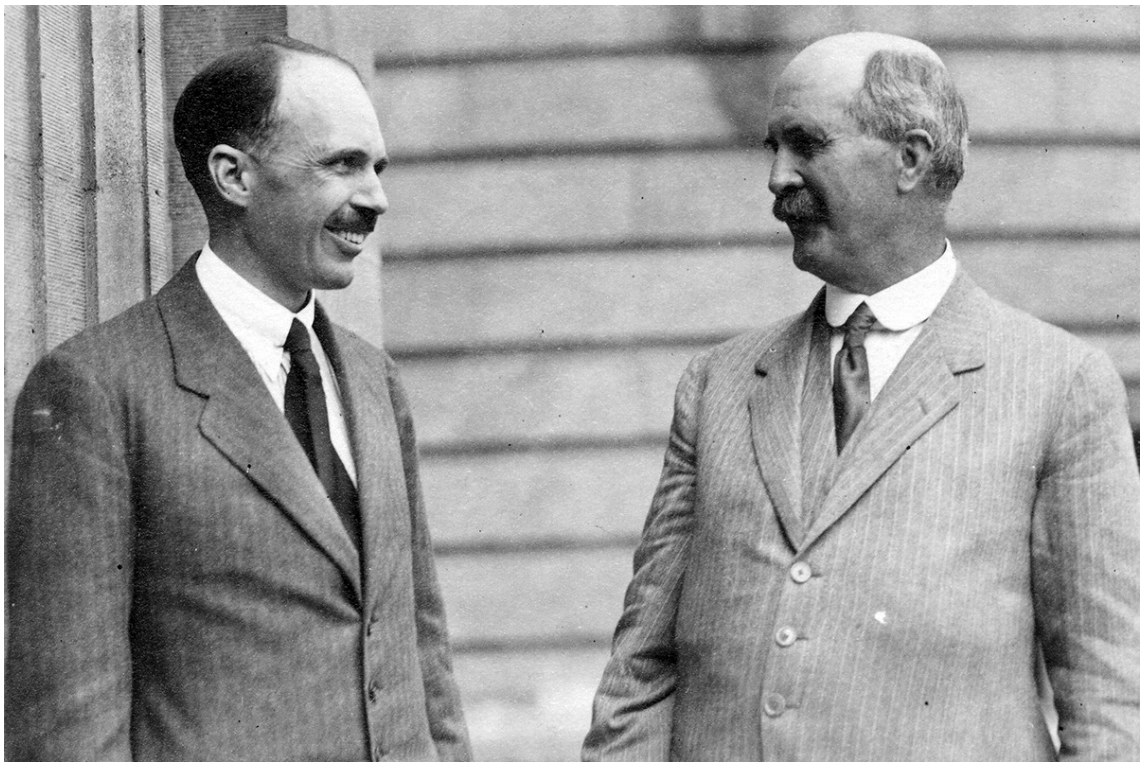
The IPC meeting on 15–16 May 2019 was held at the Hotel Olsanka, which was where all the IPC members were staying. In a departure from the agenda, it was suggested that we start by discussing and then voting on plenary lectures then keynote lectures and finally microsymposia. We had to cut the number of proposals quite substantially: plenary lectures from 26 to three, keynote lectures to 34 (about one third of all proposals) and microsymposia to 104 (about one half of all proposals). The co-chairs were not discussed in detail. After quite a lengthy preparation, the work of the IPC appeared to be efficient and we arrived at the above reductions in one and half days. The list of keynote lectures and microsymposia was approved by the IUCr Executive Committee in June 2019.

For more information on the IUCr Congress in Prague 2020, see here.

Original article: https://www.iucr.org/news/newsletter/etc/articles?issue=142706&result_138339_result_page=12

AWARDS AND PRIZES

W. H. & W. L. Bragg Prize



William Lawrence Bragg (left) and William Henry Bragg. Credit: Smithsonian Institution Archives. Image # SIA2007-0340.

In 2017 the IUCr established a prize in the name of the father and son team William Henry and William Lawrence Bragg, who pioneered the scientific discipline of X-ray crystallography, and shared the Nobel Prize for Physics in 1915. W. L. Bragg was only 25 at that time and he remains the youngest Nobel Prize recipient in any scientific discipline.

Although most scientific awards are made to well-established scientists, the W. H. & W. L. Bragg Prize will be awarded to up to two promising early-career crystallographers. This is very much in line with the characters of the two Braggs, who actively encouraged young scientists, both women and men without discrimination, to pursue a career in crystallography. Their encouragement resulted in many young crystallographers achieving considerable distinction, including the Nobel Prize winners Dorothy Hodgkin, Max Perutz, John Kendrew, Francis Crick and James Watson.

The W. H. & W. L. Bragg Prize will be awarded at IUCr Congresses, the first in 2020 in Prague, Czech Republic. The awardee(s) will receive a certificate and a financial reward, and will be invited to make a presentation at the Congress on a topic related to the prize citation.

Research achievement relative to opportunity will define the eligibility of candidates for this award. For this purpose an “early-career researcher” is defined as one who received their PhD no more than 10 years before the closing date for nominations. Academic interruptions, including periods of parental leave, will be taken into account if clearly

indicated in the letter of support accompanying the nomination. A current Curriculum Vitae and relevant details of the nominee's research publications should also accompany the nomination. The Selection Committee is as follows:

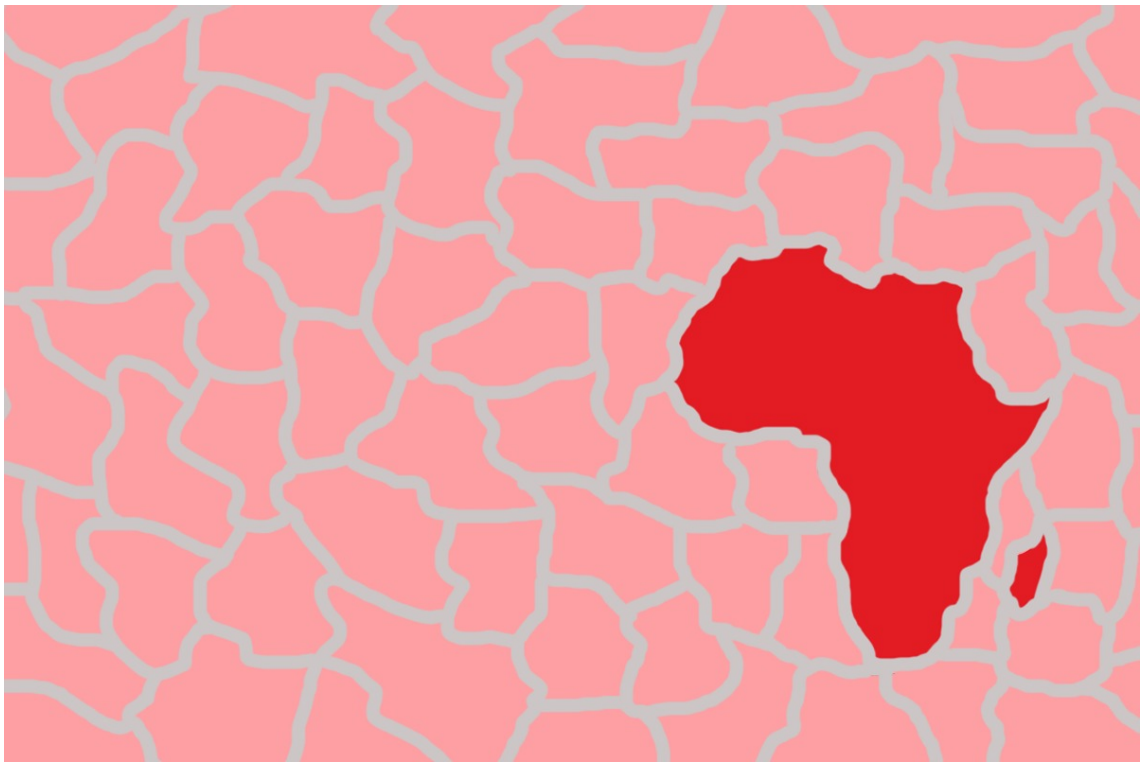
> Elena Boldyreva, Chair (Russia)
>
> Susan Bourne (South Africa)
>
> Kenneth Harris (UK)
>
> Cora Lind (USA)
>
> Mark Spackman (Australia)
>
> Michiyoshi Tanaka (Japan)
>
> Manfred Weiss (Germany)

More information about making a nomination for the First W. H. & W. L. Bragg Prize is available here.

Original article: https://www.iucr.org/news/newsletter/etc/articles?issue=142706&result_138339_result_page=13

Laying the foundations for the future: The African Crystallographic Association

Delia HaynesMarielle AgbahoungbataPatrice Kenfack Tsobnang



Africa is a continent full of potential. It has the world's youngest population and abundant natural resources despite being the world's poorest and most under-developed continent. The growth of science and technology in Africa is crucial in order to develop this huge potential and to lead to lasting change in the lives of its 1.2 billion inhabitants. Crystallography underpins so many sciences and could thus be a vehicle for this change. The development of crystallography in Africa will promote scientific cooperation between the continent's 54 countries, as well as provide solutions to many of its pressing problems in areas such as pharmaceuticals, agriculture, value-added materials and mining.

Currently, Algeria, Cameroon, Egypt, Morocco, South Africa and Tunisia are represented at the IUCr by adhering bodies. However, there are practitioners of crystallography in many other African countries. To enhance communication between crystallographers in Africa, and to grow expertise in the field, the idea of an African Crystallographic Association arose.

Background

The IUCr Crystallography in Africa initiative, launched in 1999 following a proposal by Jan Boeyens and presently chaired by Claude Lecomte, has for some time been working to promote the development of crystallography in Africa. During the International Year of

Crystallography in 2014, one of three IUCr-UNESCO summit meetings was held in Bloemfontein in South Africa. The summit, organised by André Roodt with the theme 'Crystallography as a vehicle to promote science in Africa and beyond', was preceded by a conference focussing on crystallography in Africa. One outcome of the summit was a declaration in the form of a letter of appeal for the initiation and support of regional scientific collaboration, particularly in crystallography. This letter, signed by 73 attendees at the summit, envisaged the formation of an African Crystallographic Association, AfCA. A steering committee for the formation of AfCA, chaired by André Roodt, was formed at this meeting. This consisted of representatives from nearly 30 countries across Africa. The closing ceremony of the International Year, held in Morocco in April 2015, incorporated a conference on the theme of 'Crystallography for the next generation'. At this event a letter of commitment was signed, which included resolutions to build capacity in crystallography in the developing world.



Initial signatories of the declaration arising from the Bloemfontein summit meeting. Seated from left: Patricia W. Gitari (Kenya), Habib Boughzala (Tunisia), Abdelmalek Thalal (Morocco) and Zephirin Yav (DR Congo). Standing from left: Michele Zema (IYCr2014 Project Manager at IUCr; Italy), Jean Paul Ngome-Abiaga (UNESCO; Gabon), Santiago García-Granda (IUCr; Spain), André Roodt (South Africa; organizer of the summit meeting) and Jean Ngoune (Cameroon).

Progress towards AfCA

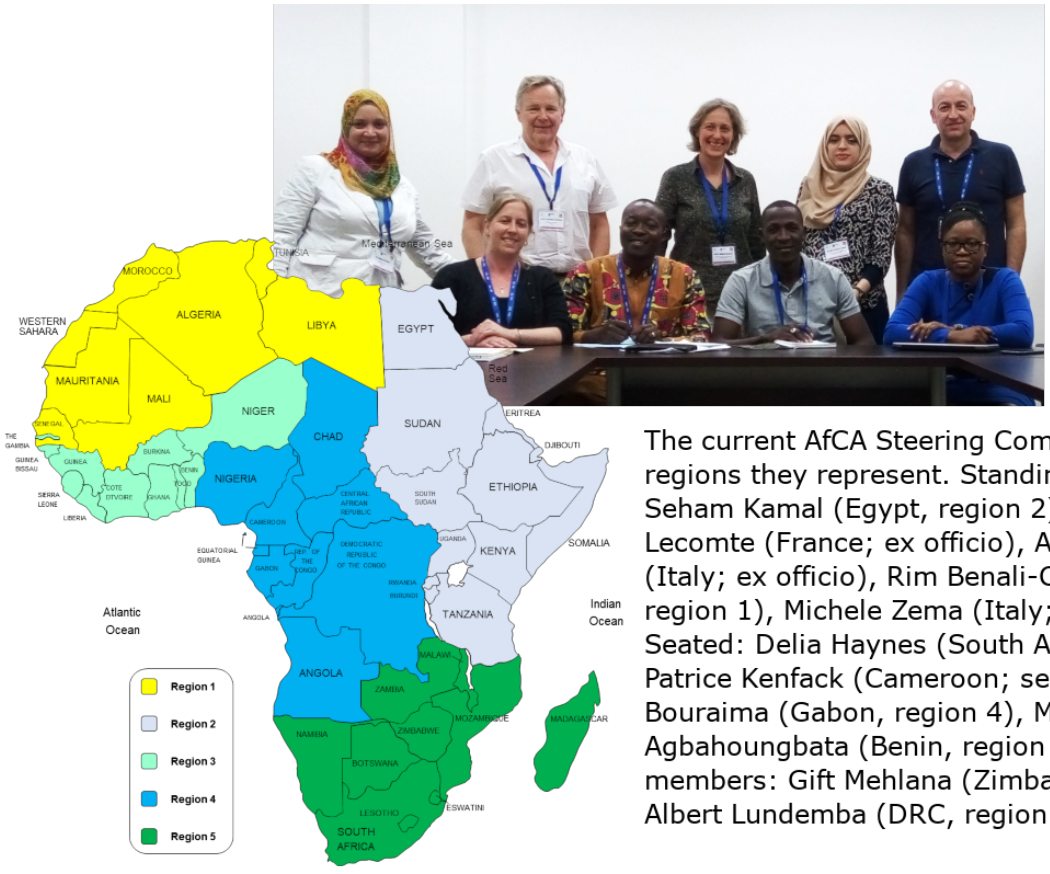
In 2016, the first Pan African Conference on Crystallography (PCCr1) was organised in Dschang, Cameroon. The theme of this highly successful conference was 'Crystallography for sustainable development in Africa'. Apart from the oral and poster communications, there were two important round tables devoted respectively to 'Crystallography as vehicle to promote science in Africa and beyond' and 'Equipment for African laboratories and the

African light source, AfLS'. During these two meetings, the path towards AfCA was discussed.

A number of African delegates attended the 24th IUCr Congress in Hyderabad, India, in 2017, at which there were two meetings related to crystallography in Africa. The first was an open session on 'Crystallography in emerging nations: Projects for a sustainable development of education and research infrastructure in Africa'. The aim was to present projects and activities related to crystallography in Africa and to highlight possible synergies among scientific unions and other bodies (UNESCO and ISC), in order to facilitate a sustainable development of education and research infrastructures in Africa. During the second meeting, the steering committee of AfCA (AfCA-SC) was restructured into its current form: a representative from each of five regions in Africa, as well as three *ex-officio* members, a chair and a secretary.

In early 2018, a conference and an OpenLab were held in Abidjan, Côte d'Ivoire, to celebrate the inauguration of a diffraction laboratory containing a single-crystal and a powder diffractometer, at Université Félix Houphouet-Boigny. This meeting saw renewed commitment to drive the formation of AfCA forward.

The second PCCr meeting was held in Accra, Ghana in January 2019. The theme of the conference was 'Crystallography, a tool for sustainable development in Africa'. The AfCA-SC members met several times during the conference, and made great progress in planning for the association. André Roodt stepped down as the chair of the steering committee, and Delia Haynes was chosen as the new chair. Several new members of the AfCA-SC were also appointed, including Rim Benali-Cherif and Gift Mehlana.



The current AfCA Steering Committee, with the regions they represent. Standing (l-to-r): Seham Kamal (Egypt, region 2), Claude Lecomte (France; ex officio), Alessia Bacchi (Italy; ex officio), Rim Benali-Cherif (Algeria, region 1), Michele Zema (Italy; ex officio). Seated: Delia Haynes (South Africa; chair), Patrice Kenfack (Cameroon; secretary), Adam Bouraima (Gabon, region 4), Marielle Agbahoungbata (Benin, region 3). Other members: Gift Mehlana (Zimbabwe, region 5), Albert Lundemba (DRC, region 4).

The path forward

Since PCCr2, the AfCA-SC has launched a Facebook page for AfCA, which provides a forum for discussion as well as dissemination of information. There is also an active WhatsApp group of young crystallographers in Africa, which arose from a crystallography school in Sénégal. Social media is playing an important role in keeping crystallographers in touch with each other across our vast continent!

Significant progress has also been made in developing a database of practising crystallographers in Africa, as well as a list of equipment. The AfCA-SC members have contacts in most African countries, and this network is used to distribute information.

A formal bid process led to the selection of Kenya as the host of PCCr3 in 2021. We plan to formally launch AfCA at this meeting. The AfCA-SC is currently working hard on developing statutes for the new association, as well as supporting the formation of regional crystallographic societies representing various countries.

A vision and mission for AfCA has been developed out of the declaration signed at the Bloemfontein summit in 2014:

The mission of the African Crystallographic Association is to contribute to the advancement of science on the African continent via crystallography in all its aspects, including related topics concerning the structure and related properties of non-crystalline states, and to promote African cooperation in crystallography.

AfCA will realise its mission through actions laid out in its strategic vision. These include creating networks and establishing associations, organising PCCr meetings, supporting training activities such as schools, and OpenLabs and outreach. One significant action is to lobby for the introduction of a scientific visa to ensure mobility of researchers between African nations. This arises directly from the declaration at the 2014 summit, where obtaining visas was highlighted as a real obstacle to scientific cooperation in Africa.

The process of forming an African Crystallographic Association is gaining significant momentum. A solid foundation has been laid on which crystallographers on the continent can build in the future. It is an exciting time to be a crystallographer in Africa!

Original article: https://www.iucr.org/news/newsletter/etc/articles?issue=142706&result_138339_result_page=14

A great day for crystallography in Benin

Claude Lecomte



Some of the researchers who participated in the event.

On 23 May 2019, the first crystal structure of a molecule synthesized and crystallized at the University of Abomey-Calavi in Cotonou, Benin, was solved during a crystallographic training session at the X-TechLab in Sèmè City, Benin, organized within the framework of the IUCr-UNESCO OpenLab in partnership with Bruker and *LAAAMP*.

The Programme Committee of this first crystallographic training session at the X-TechLab [note: a training session on X-ray microtomography was held in parallel with the crystallography class] was chaired by Claude Lecomte (CRM^2, University of Lorraine, France) and the training staff included Professor Lecomte, Patrice Kenfack (University of Dschang, Cameroon), Florence Porcher (CEA Saclay, France), El-Eulmi Bendeif and Emmanuel Wenger (CRM^2, University of Lorraine, France), Pierre Fertey (Synchrotron Soleil, France), Michele Zema (University of Pavia, Italy) and Eddy Martin (Bruker France).

Thirty students (PhD students, researchers and professors) took part in the training session, half of whom were from Benin and the other half from Burkina Faso, Togo, Congo-Brazzaville, Senegal, Cameroon and Chad. The IUCr provided EUR5000 for bursaries. Geometric crystallography and X-ray diffraction were taught during the first week, while the second week was devoted to hands-on single-crystal (14 participants) and powder (16 participants) diffraction.

All students who attended the school path on single-crystal diffraction collaborated in the solution and refinement of the crystal structure, under the supervision of Dr Bendeif. The compound studied was 4-(morpholine-4-carbonothioyl)benzoic acid ($C_{12}H_{13}NO_3S$), a thioamide compound, in particular a morpholino(phenyl)methanethione derivative. These molecules inhibit the activity of the enzymes monoacylglycerol lipase and fatty acid amide hydrolase, with beneficial effects for anxiety, pain and neurodegenerative diseases, such as Alzheimer's disease. For more information, see the Appendix below. The research team plans to submit its findings to *Acta Crystallographica*.

Three other original structure determinations of compounds synthesized in Cameroon were performed, which are also of publishable quality even though the data were collected at room temperature.

The staff of X-TechLab, and of Sèmè City, provided us with very modern teaching equipment and we also had a Bruker D8 QUEST ECO single-crystal diffractometer equipped with the latest version of the Photon II detector at our disposal. In addition, the school benefitted from free access to the Cambridge Structural Database (CSD) and related software through the CCDC FAIRE programme, and to IUCr Journals and *International Tables for Crystallography* through the IUCr Journal Grants Fund.

The general atmosphere was excellent with a lot of interested participants who asked many questions during this two-week training session (from 9 am to 8 pm!). At the end of the school, most participants were able to solve and refine crystal structures (the single-crystal group) or analyse the powder data files (the powder group) using the best freely available software. Professor Lecomte, who is Chair of the IUCr Crystallography in Africa initiative, expressed his gratitude to the school tutors, in particular Dr Bendeif, and to Bruker.

APPENDIX

4-(Morpholine-4-carbonothioyl)benzoic acid – the first crystal structure determined in Benin

H. F. Agnimonhan, F. A. Gbaguidi and L. A. Ahoussi

Laboratory of Physics and Synthesis Organic Chemistry, Faculty of Sciences and Techniques, University of Abomey-Calavi, Cotonou, Benin

4-(Morpholine-4-carbonothioyl)benzoic acid, C12H13NO3S, is a thioamide compound, in particular a morpholino(phenyl)methanethione derivative. Some studies have shown that certain morpholino(phenyl)methanethione derivatives inhibit the activity of the enzymes MGL (monoacylglycerol lipase) and FAAH (fatty acid amide hydrolase) (Kapanda et al., 2008; Draoui, 2009). FAAH and MGL catalyze the degradation reaction of anandamide and 2-arachidonoylglycerol, respectively (Mechoulam *et al.*, 1995), which are endocannabinoids with beneficial effects in pathophysiological phenomena such as anxiety, pain and neurodegenerative diseases (*e.g.* Alzheimer's disease) (Walker *et al.*, 2000; Scherma *et al.*, 2008; Zvonok *et al.*, 2008). In addition, we have studied other

morpholino(phenyl)methanethione derivatives for their toxicity on *Artemia salina* Leach larvae and trypanocidal activity (Agnimonhan *et al*., 2012).

We synthesized the title compound, a novel molecule, to study its pharmacological properties, and have reported the effect of the K-10 catalyst on the green synthesis approach used (Agnimonhan *et al.*, 2017). On 23 May 2019 during a crystallographic training session at the X-TechLab in Sèmè City, Benin, its crystal structure – which to our knowledge has never been studied previously – was determined by single-crystal X-ray diffraction analysis at 273 (2) K on a Bruker D8 Quest diffractometer. The compound crystallized in the monoclinic $P2_1/n$ space group.

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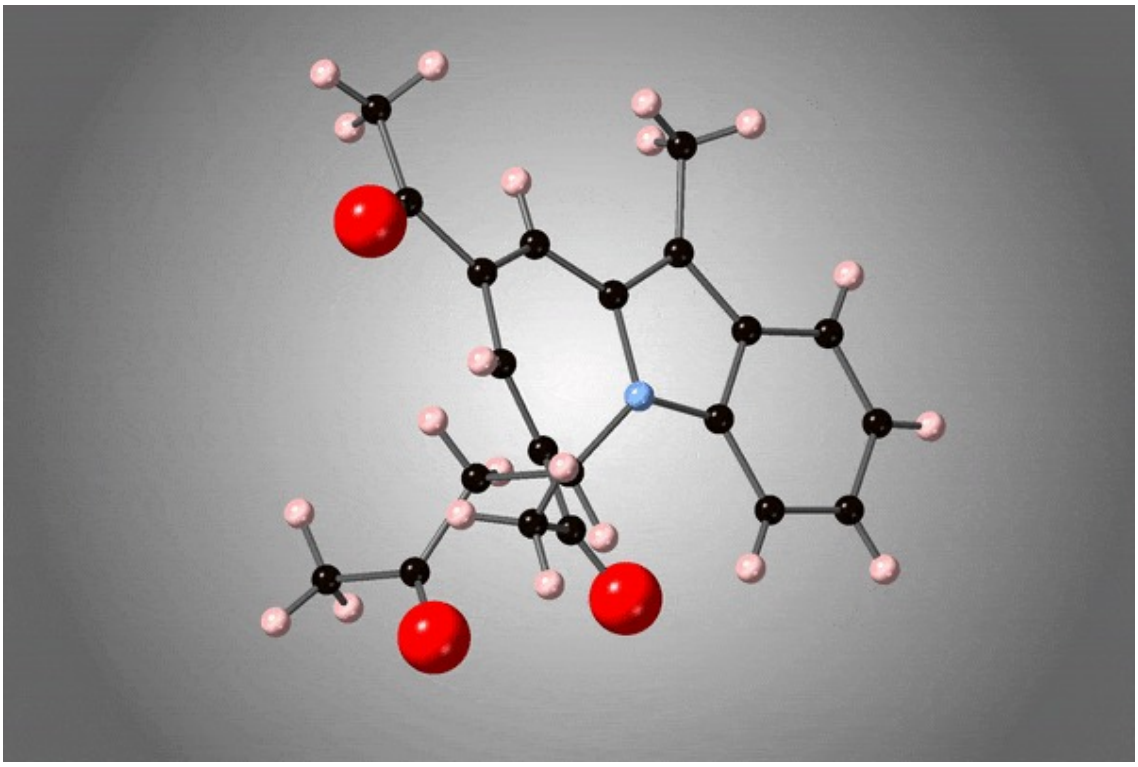
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Original article: https://www.iucr.org/news/newsletter/etc/articles?issue=142706&result_138339_result_page=15

SPECIAL REPORT

A million thanks

Suzanna Ward



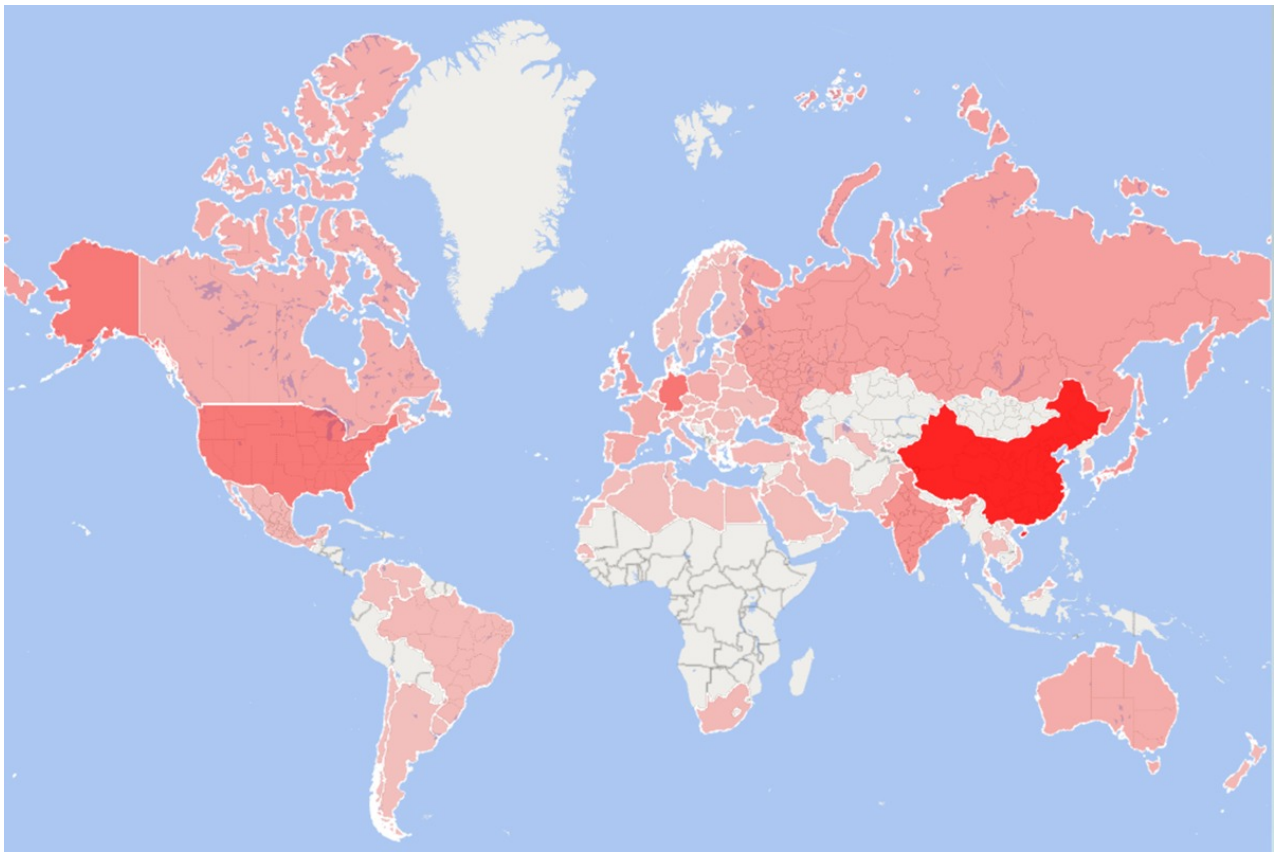
With the recent inclusion of the one millionth structure in the Cambridge Structural Database (CSD) we wanted to take this opportunity to thank you, the crystallographic community. I also thought it would be fun to reflect on how the structures published in 1965 compare with the structures published on the day we reached a million!

The sharing of one million organic and metal–organic crystal structures is an achievement of which we should all be extremely proud. Crystallographers worldwide have contributed to this achievement and without your efforts to share and publish your data this milestone would not have been possible.

The sharing of the millionth structure comes 54 years after work on the database first began. Its beginnings can be traced back to 1965 and J.D. Bernal and Olga Kennard who had the vision and foresight that the collective use of data would lead to the discovery of new knowledge, and that vision has certainly come to fruition today. Since then many people at the Cambridge Crystallographic Data Centre (CCDC) past and present have contributed to the growth and development of the CSD, scientists worldwide have deposited their data and we have been guided by our Board of Trustees who are also members of the community.

If we look at the structures published this year to date, we can see that the crystallographers responsible for the data hail from over 70 different countries. So far this year China occupies the top spot with over 25% of the structures. China is followed by

Germany, USA, India, Japan, UK, Russia, France, Australia and Spain who all make it in the top 10 countries publishing data so far this year.



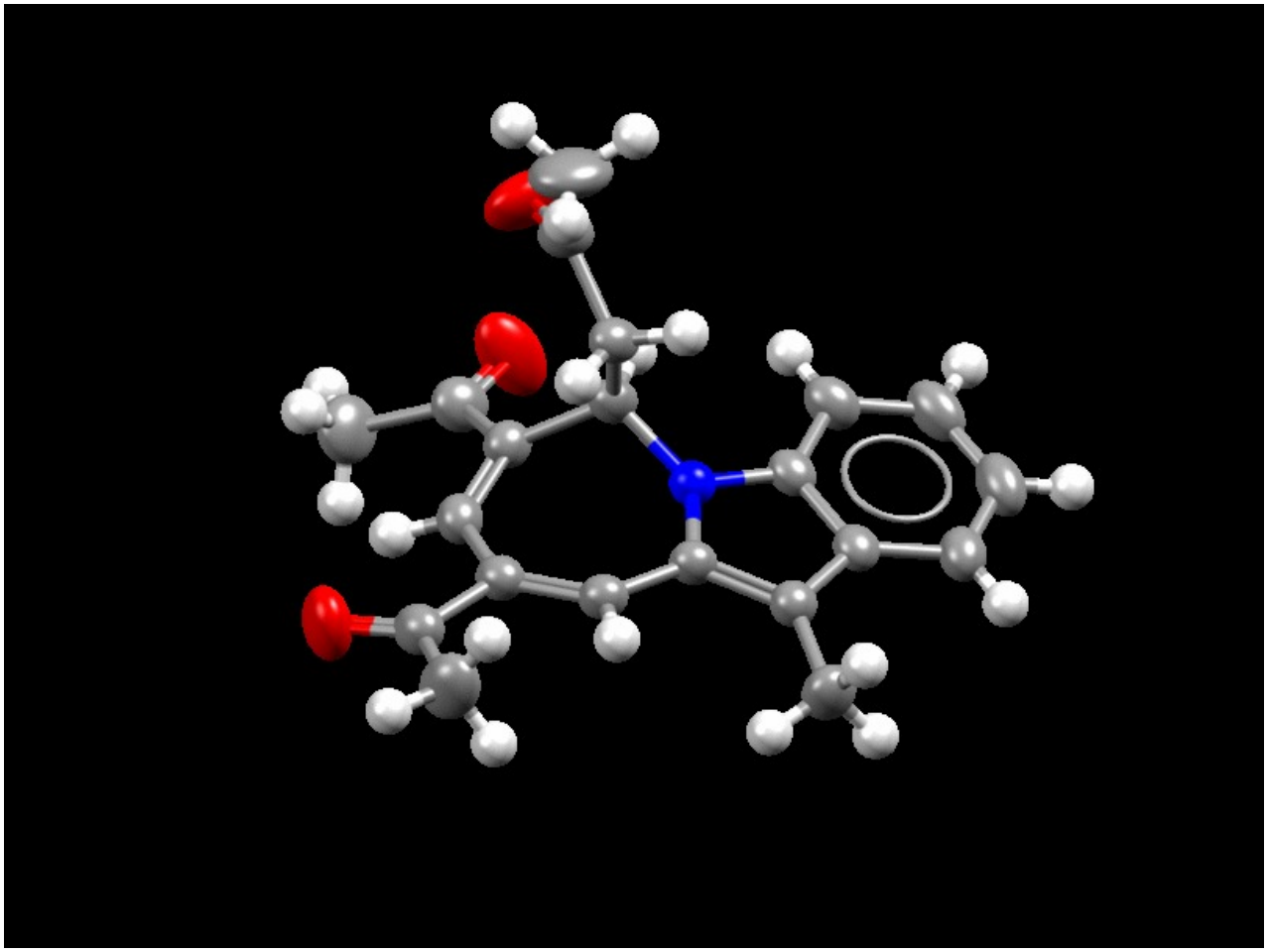
A map showing where the crystallographers are from in the structures published in the CSD so far this year (2019).

We can also look to see which crystallographers have published the most data over the years. Over 750 authors have each published more than 500 structures in the CSD. Currently Brian Skelton from the University of Western Australia is our most prolific author with over 5,800 structures. He is closely followed by Allan H. White then Arnie Rheingold, Peter Jones, Mike Hursthouse, Alex Slawin, Frank Fronczek, Judith Howard, Hoong-Kun Fun and Seik Weng Ng. We owe our sincere thanks to these authors for their contributions and to the other 350,000+ authors who have structures in the CSD. Without your efforts the CSD would not be the valuable resource it is today!



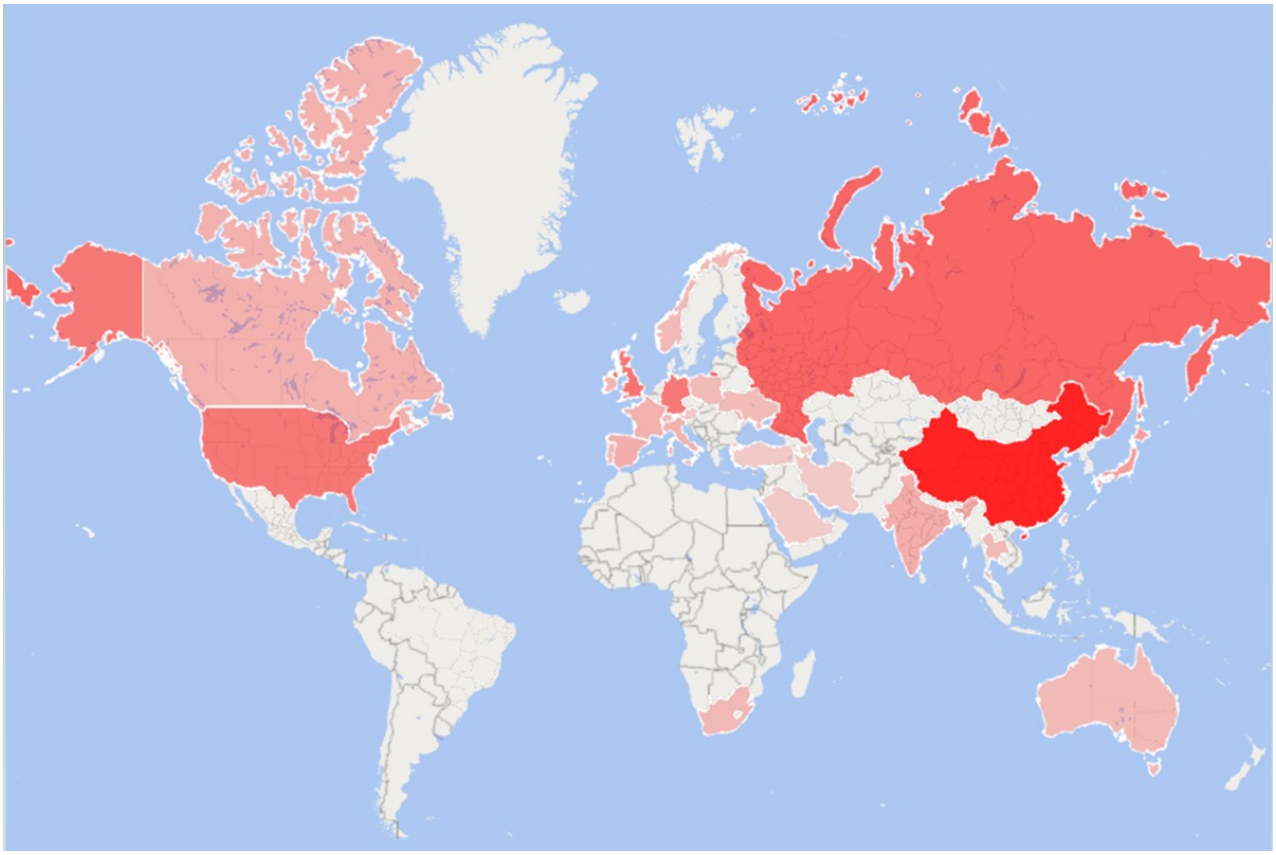
A Wordle showing the most prolific authors in the CSD.

Given the prevalence of structures from the country it is perhaps unsurprising that the millionth structure (an *N*-heterocycle) was from Yao Wang and co-workers at Shandong University, China.[1]



CSD Refcode XOPCAJ, the millionth structure added to the CSD.

On the same day that we reached one million structures, over 550 other structures were also published in the CSD. These were determined by over 170 different crystallographers so hundreds of you were tantalisingly close to being the author of the millionth! Again, if we look at where in the world these structures came from we can see that China led the way but the top 10 on #CSD1Million day saw China followed by Russia, UK, Germany, USA, Japan, India, Spain, France and Canada. So, it looks like crystallographers in some countries were slightly better at timing their publications to be in with a chance than others! Special mention should also go to Azerbaijan. According to our records there is only one structure published this year in the CSD from a crystallographer in an Azerbaijan and it was on CSD one million day so you nearly timed it perfectly! We also saw a rise in the number of *CSD Communications* published around CSD one million, as some of you tried to increase your chances of being the millionth author. In fact, 12% of the structures published on the day we reached a million were *CSD Communications*. Unfortunately for our *CSD Communication* authors the millionth structure didn't happen to be from this pool but these otherwise unpublished structures are still a valuable resource for the community and you get a full CCDC citation so don't let that put you off publishing more! For the curious among you we will be publishing a series of blogs on our website in the coming months highlighting some of the other structures that were published on CSD one million day. Keep an eye on our website and social media posts if you want to see if you got close! [2]



A map showing where the crystallographers were from on the day the CSD reached one million structures.

Intriguingly the number of structures published on the day we reached one million is nearly comparable to the number of structures published during all of 1965 when the CSD was first established. In 1965 a total of 655 structures were published and on CSD one million day a total of 588 were published in the CSD. This is an amazing feat and shows just how far crystallography and the CSD have come in the intervening 54 years. As we love looking at the data in the CSD we thought we would see how the structures published in 1965 compare with the structures published in 2019 on CSD one million day. Given the small number of structures we are comparing be warned this is purely for fun and just gives a snapshot!

In 1965 for the structures reporting a value, the average *R* factor was 6.6% compared with an average of 5.4% on CSD one million day, although for nearly a half of the structures in 1965 there is no *R* factor available so this may not be a true reflection of the change. We can also look at the study temperature and see that on CSD one million day the average study temperature is 190 K compared to 260 K in 1965 showing the rise in low-temperature studies since the CSD was first established. With so much data encapsulated in one million structures there really are endless statistics and insights to be derived from the data, some more meaningful than others! If you are interested in learning more, we now have a new CSD Statistics and Insights section on our website.[3]

I would like to finish by thanking you for sharing over one million organic and metal–organic structures. We hope that you enjoy looking at the individual structures as much as we do at the CCDC. We also hope you can continue to gain new insights and knowledge from this tremendous wealth of data. We look forward to continuing celebrating this achievement at the ACA, ECA, Fall ACS and AsCA meetings later this year.

[1] Wang, W., Zhu, H., Liu, S., Zhao, Z., Zhang, L., Hao, J. & Wang, Y. (2019). *J. Am. Chem. Soc.* **141**, 9175–9179.

[2] https://www.ccdc.cam.ac.uk/Community/blog/

[3] https://www.ccdc.cam.ac.uk/CCDCStats/

Original article: https://www.iucr.org/news/newsletter/etc/articles?issue=142706&result_138339_result_page=16

MEETING REPORT (IUCR SUPPORTED)

ESCG2 and ECCG6

Bogdan RanguelovMichail MichailovVessela Tsakova



ESCG2 participants.

European Conferences on Crystal Growth (ECCG) and the satellite European Schools on Crystal Growth (ESCG) are organized every three years under the supervision of the European Network of Crystal Growth (ENCG) and local key representative organizations in the field. They are also supported by the International Organization on Crystal Growth.

ESCG2 and ECCG6, which took place at the Riviera Holiday Club, Varna, Bulgaria, from 13 to 20 September 2018, were organized by Bogdan Ranguelov, Michail Michailov and Vessela Tsakova (Institute of Physical Chemistry, Bulgarian Academy of Sciences, Sofia, Bulgaria) together with Andrea Zappettini (IMEM, Parma, Italy) and Pierre Müller (CINaM, Aix-Marseille University, France). The two scientific events were dedicated to the famous Bulgarian scholar Iwan N. Stranski. Professor Stranski (1897–1979) played a crucial role in the last century in setting up the theoretical fundamentals of nucleation and crystal growth phenomena.

The lecture topics of ESCG2 and the scientific program of ECCG6 were structured in a way that included diverse aspects of crystal growth, crystallization and crystallography too, trying to cover the mutual interconnection between these important subjects, and thus encouraging the multidisciplinary approach to scientific problems closely related to the demands of society in different areas of modern life.

ESCG2 lectures included *Classical Approach of Crystal Growth* (Andrey Milchev, Institute of Physical Chemistry, Bulgarian Academy of Sciences, Sofia, Bulgaria), *Statistical Physics and Mechanisms of Crystal Growth* (Pierre Müller, CINaM, Aix-Marseille University, France), *Bulk Growth Methods* (Roberto Fornari, University of Parma, Italy), *Protein Crystallization* (José Gavira, National Research Council CSIC, Granada, Spain), *Multiscale Modelling of Crystal Growth* (Daniel Vizman, West University of Timisoara, Romania), *Fundamentals of Vapour Growth and Epitaxy* (Geoffroy Prévot, Paris Institute of Nanosciences, France) and *Monolayer Material Growth* (Matteo Bosi, IMEM-CNR, Parma, Italy).



ESCG2 lecturers.

The total number of ESCG2 participants was 59. Fifteen young researchers/PhD students who took part in both the school and conference received IUCr grants to partially cover travel and/or accommodation expenses.

The ECCG6 scientific program took place over 11 sessions that covered all contemporary aspects of crystal growth science: *Fundamentals of Nucleation and Crystal Growth* (Chairs: Dimo Kashchiev and Elias Vlieg); *Bulk Crystal Growth* (Chairs: Thierry Duffar and Daniel Vizman); *Surfaces, Interfaces, Epitaxial Growth, Thin Films* (Chairs: Knut Deppert and Michal Leszczynski); *Structural Defects and Impurities in Crystalline Materials* (Chairs: Andreas Danilewsky and Bogdan Ranguelov); *Crystal Growth and Characterization of Nanostructures, Low-dimensional and Confined Systems* (Chairs: Vladimir Dubrovskii and Michail Michailov); *Crystallization of Inorganic Materials* (Chairs: Alberta Bonanni and Linda Pastero); *Crystallization in Organic and Biological Systems* (Chairs: Giuseppe Falini and Stéphane Veesler); *Industrial Crystallization, Technologies and Process Control* (Chairs: Heike Lorenz and Kevin Roberts); *Novel Materials and Structures* (Chairs: Raffaella Lo Nigro

and Dorota A. Pawlak); *New Methods and Techniques for Crystal Growth* (Chairs: Christiane Frank-Rotsch and Evgeny Zharikov); and *Advances in Observation and Characterization Methods* (Chairs: Florinda da Costa and Ionut Enculescu).

Altogether, two plenary talks, 26 invited lectures, 35 oral talks, two memorial lectures and more than 200 poster presentations were included in the ECCG6 program. The total number of ECCG6 participants was 260. Ten young researchers/PhD students (not involved in ESCG2) received IUCr grants to partially cover travel and/or accommodation expenses. Thus, 25 IUCr grants were given in total.

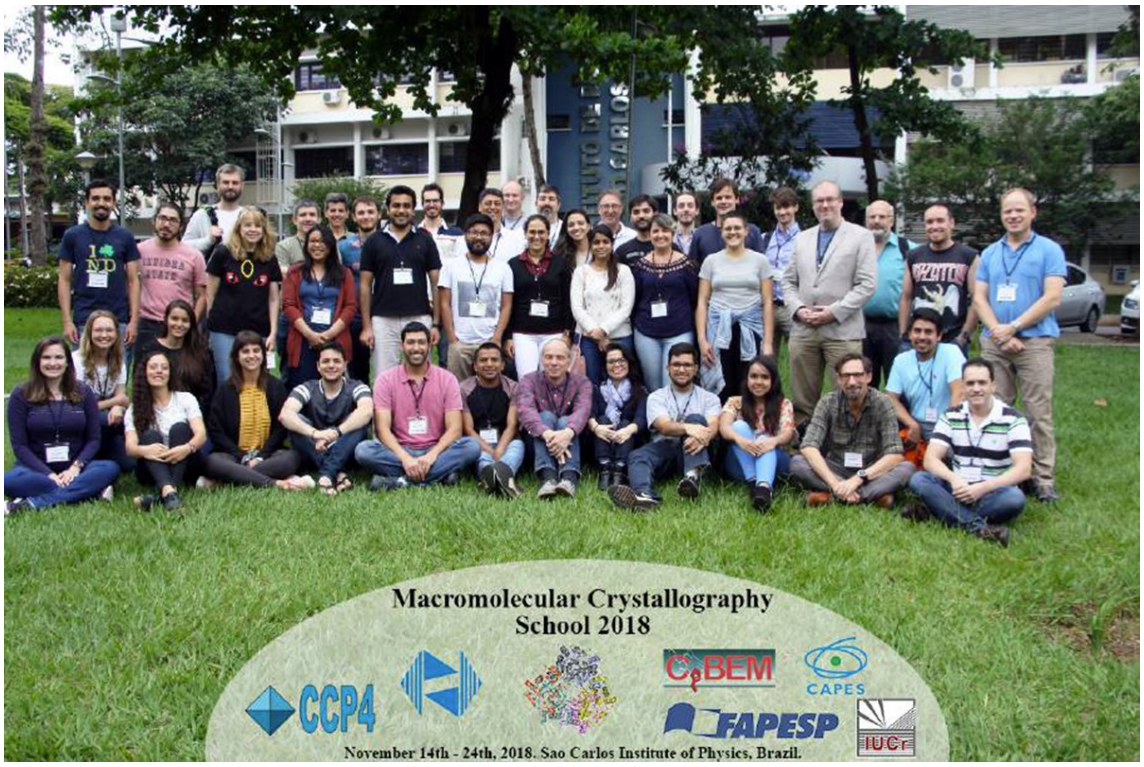


IUCr-supported ESCG2 participants.

Original article: https://www.iucr.org/news/newsletter/etc/articles?issue=142706&result_138339_result_page=19

MEETING REPORT (IUCR SUPPORTED)

Macromolecular Crystallography School 2018



Group photo with teachers and students.

The Macromolecular Crystallography School "From data processing to structure refinement and beyond" was held at Sao Carlos Institute of Physics, University of Sao Paulo, Brazil, from 14 to 24 November 2018, and organized by João R. C. Muniz, Richard Garratt and Glaucius Oliva from the Sao Carlos Institute of Physics, and Kyle Stevenson and Ronan Keegan from STFC Rutherford Appleton Laboratory, Oxfordshire, UK. This workshop represents the continuation of the series that started in 2010 at the Institut Pasteur de Montevideo, Uruguay. As for the previous four editions in Uruguay and Brazil, the 2018 workshop was co-organized with the Collaborative Computational Project Number 4 (CCP4 - UK). We invited 18 teachers and tutors, gathering a group of leading experts in developing cutting-edge methods for protein crystallography and structural biology.

From 65 applications, we selected 24 students from seven different countries (Brazil, Mexico, Argentina, Chile, India, South Africa and UK). The oversubscription forced us to decline many good applications but it revealed that there is a need to keep this course running. Its visibility at the international level has become well established. The attendees were mostly advanced PhD students, postdocs and a few young research scientists. The idea in this respect was to prioritize people who could put this training into use in concrete research work as fast as possible.

During the workshop, lecturers guided the students through dedicated tutorials covering the main programs and state-of-the-art algorithms in macromolecular crystallography. The

workshop was conceived to provide a strong theoretical background in the form of lectures, and hands-on abilities (problem-solving sessions) in the use of computational tools to exploit X-ray diffraction data (mostly brought by the students) and datasets with varying degrees of difficulty were also provided to students who did not bring their own. Particular emphasis was given to data processing, phasing/structure determination and model refinement/validation, also including, for the first time, sections on electron microscopy.

The course covered the following topics:

- Data processing, particularly regarding its importance in successful structure solving;
- Phasing: basic concepts, main approaches;
- Molecular replacement;
- Experimental phasing, especially regarding the use of anomalous diffraction;
- Macromolecular model refinement: target functions, minimization algorithms, main programs;
- Data and model validation;
- Cryo-EM: structure building, refinement, and map fitting.

English was used throughout the course. Lectures were mainly scheduled in the mornings, with tutorials and hands-on practical classes in the afternoons. Practical classes were aimed at solving genuine problems brought in by the students (starting from the students' X-ray diffraction data). Experimental data were assigned by the local organizers to the few students who had not brought their own data, so they could follow the tutorials and attempt to solve the structures during the problem-solving sessions. Two "Burning questions" sessions, as well as poster presentations (based on the students' scientific research projects), reinforced active discussion times; the posters were on display during the whole course.

The Sao Carlos Institute of Physics is well equipped for practical structural biology courses. The Protein Crystallography Unit gives access to a state-of-the-art X-ray home source to perform single-crystal diffraction experiments under cryogenic temperatures, and other units in the institute allow for recombinant protein production/purification as well as in-solution biophysical characterizations.

It is important to highlight that most of the computational programs used during the workshop, many of them being the most widely used throughout the international macromolecular crystallography community, were taught directly by the program developers themselves, constituting a unique opportunity for intense and productive interaction. The aims of this workshop have been kept coherent since the first course in 2010, contributing to the explicit interest in consolidating continuity in a local Macromolecular Crystallography School. At the same time, we have clearly moved forward in incorporating improvements, and in keeping up to date with the latest developments in cutting-edge methods, thanks to the expertise of the participating teachers. This fulfils an urgent need to train young scientists in this discipline. This type of workshop not only allows solid training in theory and applications in biological crystallography but also fosters collaborative, interdisciplinary and inter-institutional research programs,

consolidating regional networks in structural biology like the Center for Structural Biology of Mercosur (CeBEM).

The commitment of the teaching staff with the whole endeavour was outstanding, and the overall evaluation of the course was extremely positive. The social events accompanying the course - several dinners, the poster session, rafting in Brotas (a popular tourist attraction close to Sao Carlos) and the final barbecue - were very much appreciated and provided additional opportunities for informal interactions and discussions. Support from the Sao Carlos Institute of Physics, CeBEM, IUCr, Sao Paulo Research Foundation (FAPESP), CCP4 and the Coordination for the Improvement of Higher Education Personnel (CAPES) is greatly acknowledged.

For the 2020 edition, we are planning to put forward a web-based tool for interaction and dissemination of material and information, using the Moodle platform. We are also planning to include a final exam (optionally anonymous).

Original article: https://www.iucr.org/news/newsletter/etc/articles?issue=142706&result_138339_result_page=23

MEETING REPORT (IUCR SUPPORTED)

15th Conference of the Asian Crystallographic Association

Christopher SquireKurt Krause, Ted BakerSally Brooker



Recipients of IUCr Young Scientist Awards flanked by LOC Co-Chair Kurt Krause (left) and AsCA President Jenny Martin.

The 15th Conference of the Asian Crystallographic Association (AsCA) was held in Auckland, New Zealand, from 2 to 5 December 2018, in association with the 32nd meeting of the Society of Crystallographers in Australia and New Zealand (SCANZ). The conference venue, at the University of Auckland, proved to be an outstanding one, with excellent lecture theatres and very good spaces for delegates to mingle, and for interaction with each other and with the sponsors.

The conference attracted an impressive total of 477 registrants from 28 countries, with very pleasing attendances of scientists from Japan (86), China (47), Taiwan (29), Korea (34), India (19) and other Asian countries. Included in the attendees were 20 young scientists supported from IUCr funding.

The scientific programme included Plenary lectures by David Eisenberg (USA), Susan Lea (UK), Cameron Kepert (Australia) and Amy Rosenzweig (USA); that by Professor Eisenberg, "Proteins on the Edge: Amyloid Formation in Health and Disease", was opened to enable members of the public to attend. Keynote lectures were given by Yanli Wang (China), Hiroshi Kitagawa (Japan), Richard Neutze (Sweden), Catherine Day (New Zealand), Deanna D'Alessandro (Australia) and Ayana Sato-Tomita (Japan). The meeting opened with a

special lecture on “Crystallography as seen through the lens of the Nobel Prize” by Anders Liljas (Sweden) and concluded with a Rising Stars Symposium featuring six outstanding young scientists from Australia, Japan, India, Pakistan and New Zealand. The general programme was organised into three parallel streams of six microsymposia each, broadly subdivided into Biological Crystallography (including cryo-EM), Chemistry and Materials, and Advanced Methods.

A very enjoyable conference dinner, sponsored by Rigaku and preceded by a traditional Maori welcome, was held in a spectacular venue at the Auckland Museum, situated on the flank of one of Auckland’s volcanic cones, and looking out over the harbour and beyond.

Original article: https://www.iucr.org/news/newsletter/etc/articles?issue=142706&result_138339_result_page=24

MEETING REPORT (IUCR SUPPORTED)

Interest in data flourishes at AsCA

Amy Sarjeant



Speakers and Chairs (left to right): Amy Sarjeant (Co-Chair), Stephen Burley, James Hester, Matthew Lightfoot, Janet Newman, Brian McMahon, Takeshi Kawabata and Genji Kurisu (Co-Chair).

Late last year I had the pleasure of traveling to Auckland, New Zealand, to attend the 2018 meeting of the Asian Crystallographic Association (AsCA). I'm sure this won't be the only update about this excellent conference, but I wanted to take this opportunity to write a short summary of the session I co-chaired with Genji Kurisu of PDBj. Early on in 2018, we had been asked to chair a session entitled "Database developments, validation and data mining." This was the first time a session devoted solely to databases was included as part of the program for the AsCA meeting series. As our community continues to tackle the issues surrounding data sharing under the FAIR principles (Findable, Accessible, Interoperable and Reusable), sessions like this will play an important role in outlining our response to these challenges. For our session, we were fortunate to be able to include a variety of talks from a truly international set of speakers. Topics ranged from understanding the nature of a dataset itself, to data validation and everything in between. James Hester of ANSTO kicked off the session by posing the question "What is a dataset?" As crystallographers we use the word "dataset" constantly, but often without pondering its meaning. James walked us through an approach to mapping raw image data files to imgCIF format, thereby providing a protocol for systematic raw data archive and sharing. From there, Janet Newman of the CSIRO Collaborative Crystallisation Centre (C3) took us on a tour of C6 (Comparison of Crystallization Conditions @ C3). She highlighted some of

the challenges in standardizing crystallization screen data and some of the tools her team is making available to analyse crystallization results.

The next two presentations provided updates and insights into the status of the Cambridge Structural Database and the PDB. Matthew Lightfoot of the CCDC detailed some of the work his team has been doing in understanding the quality of datasets deposited with CCDC and improving data validation through the deposition workflow. Stephen Burley of the RSCB PDB detailed the efforts of his team to identify and correct ligand refinements in PDB structures. Toward the end of his presentation, Stephen highlighted the impact of the PDB on drug approvals by the US Food and Drug Administration. Continuing with updates from the PDB, Takeshi Kawabata of the Institute for Protein Research, Osaka University, provided a look at what PDBj is doing with data from electron microscopy (EM) studies. Takeshi detailed the EMPIAR archive of raw 2D EM images as well as EM Navigator, which provides a user-friendly interface to the EMDB server.

Finally, the session concluded with a contribution from Brian McMahon of the IUCr entitled “The element of trust: validating and valuing crystallographic data.” Brian’s presentation touched on the utility of the CIF file not only as a means of sharing data but also as an enabler for data checking and validation. This talk underscored the importance of focusing on data-sharing practices and protocols, which stood at the heart of every presentation. Without standardization, we lack the ability to validate the data we are using. And without the validation, what can we truly say about the scientific conclusion we draw from these collections of data?

Sessions on data management and archive provide a forum for concerned researchers to share experiences and agree on standard practices. As members of the structural science community, we have a responsibility to provide the highest quality data achievable from our experimental studies. I would encourage everyone to look through the talks described above on the IUCr website to learn more about ongoing efforts throughout the crystallographic community.

Original article: https://www.iucr.org/news/newsletter/etc/articles?issue=142706&result_138339_result_page=25

MEETING REPORT

Future developments of advanced light sources in Latin America and the Caribbean

Abel Moreno



Panelists at the *LAAAMP* session at the CiLAC Forum 2018. From left to right: Michele Zema, Abel Moreno-Cárcamo, Richard Garratt, Graciela Díaz de Delgado, Diego G. Lamas and Carlos Cabrera-Martínez.

Since ancient times, humans have been fascinated by the beauty of crystals, their magic geometry, their intriguing shape, the existence of right angles and so on. These shapes have influenced the human mind, which has been most evident in the architecture of many buildings, skyscrapers and modern museums worldwide. During the second half of the 19th century, the architecture of many buildings was influenced by classical Greek architecture. However, at the beginning of the 20th century, the ideas of the Art Deco movement were expressed in the shape of large buildings. Later on, the Art Nouveau revival led to nonsymmetrical and curved constructions. But recently, it seems to be that modern architecture and the way that large buildings are being constructed are again being influenced by the shape of crystals.

Recently, I had the opportunity to visit Panama City on the occasion of the Open Forum for Science in Latin America and the Caribbean (CiLAC 2018), which took place on 22–24 October 2018. I was one of the panelists at the *LAAAMP* thematic session on 'Implementing Advanced Light Source facilities in Latin America and the Caribbean for sustainable socio-economic development', together with Michele Zema, IUCr Executive Outreach Officer (University of Pavia, Italy); Carlos Cabrera-Martínez (University of Puerto

Rico, USA); Graciela Díaz de Delgado (Universidad de los Andes, Mérida, Venezuela); Diego G. Lamas (National University of San Martín, Argentina) and Richard Garratt (Universidade de São Paulo, Brazil).

During a break from the sessions, we walked along the most important streets in this beautiful Central American city. After a few blocks, a wonderful building came to our attention; it was perfectly shaped in the form of a screw axis (see below left) and it made us say altogether '*Crystallography is everywhere, even in Panama City*'. This kind of building also reminded me of the Bankia building in Madrid, which has an orthorhombic shape, as well as others that resemble quartz crystals (below right).





Getting back to the CiLAC forum, we had a fantastic opportunity to discuss future developments of advanced light sources in the Latin America and the Caribbean region, and it was indeed great that such an important and strategic conference featured topics like synchrotron radiation and crystallography. For this, M. Zema and the whole *LAAAMP* Executive Committee have to be thanked for writing a good proposal and following up on their previous participation in the World Science Forum 2017 in Jordan. The CiLAC forum is a key regional space for debates and exchanges organized every two years in different cities of the region. It seeks to be a platform for outlining common positions and debating the scientific, technological and innovation agenda supporting sustainable development whilst simultaneously giving the region a strong voice in the global scope of the World Science Forum.

Our session was moderated by M. Zema, who started his opening speech with the most precise description I had ever heard about synchrotron radiation and advanced light sources, saying: '*Synchrotron light sources are the most sophisticated example of an open and multidisciplinary research infrastructure. They are comparable to supermicroscopes that probe the inner structure of matter. They produce very intense pulses of light, with wavelengths and intensities that allow detailed studies of objects ranging in size from human cells to viruses and proteins, down to atoms, with a precision that is not possible by other means. They allow researchers to investigate the structure and properties of a wide range of materials, from proteins – to provide information for designing new and better drugs – to probing novel materials for biotechnology, analyzing soils for green agriculture, to engineering applications, and the examination of archaeological artefacts*'.

Most of the discussions were concentrated on the construction of synchrotron facilities in Latin American countries, such as Mexico, Puerto Rico and Cuba. The session was focused

on discussing showcases and how advanced light sources successfully contributed to the socio-economic development of countries and regions, with particular reference to the Brazilian and SESAME experiences, by creating international scientific communities, improving education and creating new job opportunities.

In my contribution, I outlined a recent initiative of the Mexican Government to construct a synchrotron facility in the State of Hidalgo in the southeast of the Mexican Republic. It would be located in the Science Park area, where many industries and research centers have settled. Times of economic crisis are in reality times of many opportunities. If this Mexican synchrotron comes to fruition, it will reinforce the Mexican economy and enable it to provide for better technological opportunities, as happened in Brazil at the beginning of the 1990s. Besides this initiative, there are about 80 networks in Mexico sponsored by the National Council for Science and Technology (CONACYT). One of these – the Thematic Synchrotron Radiation Users' Network (RedTULS) – sponsors postgraduate students and academics to travel to synchrotron facilities. This network has allowed scientists to be trained and cultivated in the use of synchrotrons to support challenging research, which cannot be done by conventional instrumentation located in the universities. In his presentation, C. Cabrera-Martínez described the feasibility of constructing the first synchrotron in the Caribbeans, just in Puerto Rico. There are some investors from academia and government who are very much interested in this initiative. These two facilities (Mexico and Puerto Rico), which are at the business-planning stage at the moment, will create an environment that will encourage new scientific discoveries for the new millennium based on synchrotron light sources.

After returning home from CiLAC 2018, I received the good news that the State of Hidalgo has announced plans to invest USD 25 million as a seed contribution to develop a plan for a synchrotron light source in Mexico. The Mexican synchrotron facility will be completed by 2030. The facility will cost an estimated USD 800 million and its construction will take 10 years. Mexico could become the second Latin American country to host a synchrotron facility, after Brazil.

Original article: https://www.iucr.org/news/newsletter/etc/articles?issue=142706&result_138339_result_page=20

MEETING REPORT

2018 Meeting of the Crystallographic Society of Japan

Kunihisa Sugimoto



Recipients of the 2018 CrSJ Awards with the President of CrSJ (left to right): D. Hashizume, K. Miki, Y. Sugawara (President) and T. Ikeda.

The 2018 Annual Meeting and General Assembly of the Crystallographic Society of Japan (CrSJ2018) was held on 10-11 November at the Tokyo Institute of Technology, Japan, and about 300 crystallographers participated. The meeting featured 49 oral and 96 poster presentations covering all aspects of crystallography, three award lectures, three microsymposia, a special lecture promoting gender equality, two luncheon seminars and industrial exhibitions from 10 companies/organizations. The microsymposia were titled *Application of Data Analysis by New Mathematical Methods in Crystallography*, *Chemical Bonding and Crystallography under High Pressure* and *Future Development of Protein Structural Analysis through Collaboration between Crystallography and Electron Microscopy*, and a total of 15 invited talks were given.

At the CrSJ Awards Ceremony, the S. Nishikawa Award was given to Kunio Miki (Kyoto University) for his research *Development of Protein Crystallography: from Structural Biology to Biological Structure Chemistry*, and the two Research Awards were presented to Takuji Ikeda (AIST) for his research *Powder X-ray Diffraction Analysis of Zeolites and Contribution to the Development of a Multi-purpose Pattern Fitting System* and Daishuke Hashizume (RIKEN) for his research *Characterization of Labile Chemical Bonds and Reaction Mechanisms based on Electron Density Distribution Analysis*.

Eight young scientists were honored with Poster Awards: Y. Lee (Hokkaido University), R. Tamura (Yokohama City University), T. Kato (University of Tokyo), Y. Okamoto (Tottori University), Y. Terasawa (Waseda University), T. Tsujiguchi (Tokyo Institute of Technology), T. Sasaki (University of Tsukuba) and H. Kitahara (Tohoku University).



Poster Awardees with the President of CrSJ (left to right): Y. Lee, R. Tamura, T. Kato, K. Sugawara (President), Y. Okamoto, Y. Terasawa, T. Tsujiguchi, T. Sasaki and H. Kitahara.

The Young Crystallographers Meeting 2018, a satellite meeting of CrSJ2018, was held on 9 November, also at the Tokyo Institute of Technology, and 35 researchers/students participated. This meeting is held every year to provide an opportunity for young researchers and graduate students to communicate and network with each other, especially beyond the barriers between physics, chemistry and biology, in an informal environment. This year, three lectures by H. Kasai (University of Tsukuba), H. Ohtsu (Tokyo Institute of Technology) and N. Yano (Ibaraki University) were given and a banquet was held afterwards.



Young Crystallographers Meeting 2018.



Participants in the Young Crystallographers Meeting 2018.

The full program of the meeting can be viewed here. The chair of the organization committee was M. Yashima (Tokyo Institute of Technology) and the program committee was chaired by H. Uekusa (Tokyo Institute of Technology).

The 2019 annual meeting will be held on 19-20 November 2019 at Kanazawa Bunka Hall, Kanazawa, Japan. The chair of the organization committee is M. Okuno (Kanazawa University) and the program committee is chaired by H. Okudera (Kanazawa University).

Original article: https://www.iucr.org/news/newsletter/etc/articles?issue=142706&result_138339_result_page=21

MEETING REPORT

International Workshop on Chemical Crystallography and Structural Biology

Victor KhrustalevAlex YanovskyIlia Guzei



Commemorative conference medal. The front side features Prof. Struchkov’s profile and the reverse a fragment of a scientifically significant polynuclear complex whose structure was established at the INEOS X-ray Laboratory.

Better late than never. This old adage was probably on the minds of many former colleagues and students of the outstanding Russian crystallographer, Vice-President of the IUCr from 1993 to 1995, Yuri Struchkov (1926–1995), when they assembled on 13–16 November 2018 for the Second Struchkov Meeting, the International Workshop on Chemical Crystallography and Structural Biology. This is the first time this meeting has been held in Moscow, Russia, where Prof. Struchkov lived and worked all his life. The conference continued the tradition of gathering the students and colleagues of Prof. Struchkov to share their new and inspirational scientific achievements as well as precious memories of former collaborations. The first meeting took place more than 10 years ago in Chicago, IL, USA; see *IUCr Newsletter* (2007). **15**(3), 17. The current, Second Struchkov Meeting was supported by the Russian Academic Excellence Project “5-100” and hosted by Peoples’ Friendship University of Russia (RUDN University). The conference's organizational efforts were spearheaded by the Research Institute of Chemistry and Inorganic Chemistry Department of RUDN University chaired by V. N. Khrustalev, himself a former colleague of Prof. Struchkov.

The four-day meeting attracted 150 participants from Azerbaijan, Belarus, France, Germany, Kazakhstan, Kyrgyzstan, Russia, Sweden and USA and featured 48 lectures. Two satellite events preceded the opening ceremony: a workshop on advanced structural refinement techniques by I. A. Guzei (University of Wisconsin, Madison, WI, USA) and a round-table discussion “Advances in Modern X-ray Structural Analysis” chaired by S. V. Lindeman (Marquette University, Milwaukee, WI, USA). The attendees also enjoyed a social program including a get-together reception and conference dinner, as well as a Moscow sightseeing tour for international participants.



Conference participants, named left to right. Top row: Aida Samigullina, Yuri Slovokhotov, Oleg Siidra, Inna Dubchak, Nikolai Lobanov, Ilia Guzei, Alexander Korlyukov, Alexey Bilyachenko, Alexander Novikov, Olga Bulavchenko, Dmitriy Yatsenko, Vladimir Larionov, Maria Khrenova, Fedor Dolgushin, Alexander Virovets, Sergey Lindeman, Eugenia Peresypkina. Bottom row: Daut Islamov, Victor Khrustalev, Evgeny Nazarchuk, Andreii Kritchenkov, Vakhobjon Sabirov, Bolot Sadybakasov, Susan Byram, Igor Litvinov, Asylbek Yespenbetov, Irena Akhrem, Leonid Aslanov, Georgii Bogdanov, Kyryll Suponitskii, Georgy Fukin, Olga Lindeman, Tatiana Timofeeva, Alex Yanovsky, Arkady Ellern, Olga Kovalchukova, Ruben Gerr.

On the opening day, after greetings from the Conference Organizing Committee presented by T. V. Timofeeva (New Mexico Highlands University, Las Vegas, NV, USA) and the latest announcements from the Chairman of the Struchkov Prize Panel, L. A. Aslanov (Moscow State University, Moscow, Russia), plenary lectures by I. A. Litvinov (Arbuzov Institute of Organic and Physical Chemistry, Kazan, Russia) and S. K. Byram (Bruker AXS Inc., Madison, WI, USA) gave historic accounts of Prof. Struchkov’s role in the development of organic crystal chemistry as well as the spread and proliferation of crystallographic instrumentation in the Soviet Union and, later, Russia. Subsequent lectures in the first three days were primarily delivered by former colleagues of the Institute of Organoelement Compounds (INEOS) X-Ray Laboratory, founded by Prof. Struchkov in the 1970s. The talks encompassed many scientific areas, illustrating the scope of modern day studies of members of Prof. Struchkov’s school. The speakers offered serious scholarly assessments of the state of diverse subjects, mostly constructed along the then-*vs*-now model. Most presenters also took the opportunity to offer personal historical insights and a good measure of nostalgic reminiscences, which always elicited vivid reactions from the understanding audience. The majority of the participants share more than common scientific interests and memories; they regularly make contributions toward the financial and organizational support for the Struchkov Prize, an annual award bestowed upon a young Russian scientist for the best work in a field related to crystallography. This prize was established soon after the untimely death of Prof. Struchkov, see *IUCr Newsletter* (2000). **8**(4), 18, and awarded for the 22nd time in the fall of 2018. Many of the award

laureates have become well-known scientists and leading authorities in their respective fields ranging from inorganic chemistry to biology and engineering. Their impressive achievements were highlighted on the fourth day of the conference in a special session featuring talks by the former Struchkov Prize winners. All the speakers at the Conference received commemorative medals (see photo at the beginning of the article).

The particulars of the conference, including the book of abstracts, are available here.

The participants and, perhaps even more importantly, organizers closed the conference with a firm commitment to make it a regular event happening at least every 3–5 years. The organizers overcame many financial and logistical difficulties to hold this truly remarkable meeting. We are confident that the Struchkov Prize Society will build on this success and that the next meeting will eventually happen.

Donations to the Struchkov Prize Association [501(c)(3) charitable organization] are welcome. The full amount of all contributions (100%) is deposited in the Struchkov Prize fund, and subsequently awarded to the Struchkov Prize competition laureates. If you wish to make a tax-deductible contribution, please contact Alex Yanovsky.

Original article: https://www.iucr.org/news/newsletter/etc/articles?issue=142706&result_138339_result_page=22

MEETING REPORT

2018 Jana Modulation Workshop

Diane DickieMilan Gembicky



Nearly 30 crystallographers from academia, industry and government labs recently gathered for the 2018 *Jana* Modulation Workshop organized and hosted by Milan Gembicky and Curtis Moore of the University of California, San Diego, USA. The workshop was led by Václav Petříček and Michal Dušek of the Czech Academy of Sciences, two of the co-authors of the *Jana2006* software. The participants came from a wide variety of backgrounds including chemistry, geology and materials science, and their experience level ranged from graduate students to emeriti faculty. More than half a dozen US states, two Canadian provinces and three other foreign countries were represented.

Workshop participants were introduced to the *Jana2006* software and to the concept of modulation through a combination of lectures and step-by-step activities that they worked through on their own computers individually or in pairs. To familiarize themselves with *Jana2006*, the attendees first learned how to solve and refine non-modulated structures from both single-crystal and powder data. As they gained confidence and experience, more advanced concepts were introduced to the exercises. By the end of the four-day workshop, which ran from 10 to 13 December 2018, participants were modeling twins and various modulation functions, and visualizing the results in *Diamond* and *Vesta*. Everyone was sent back to their universities or companies with several more datasets to continue practicing.

In order to make sure that participants had all the necessary tools to generate and process their own datasets in the future, several other software packages were also demonstrated and distributed during the workshop. Jim Britten of McMaster University, Hamilton, Canada, gave a lecture on *Max3D*, a powerful program for visualizing reciprocal space in three dimensions. Because *Jana2006* can handle data from virtually any diffractometer, Bruce Noll of Bruker AXS and Eric Reinheimer of Rigaku Americas each gave lectures to demonstrate best practices for collecting and processing crystallographic data using the *APEX3* and *CrysAlis*^{PRO} software suites, respectively. Dr Gembicky reinforced the message of their lectures - the importance of proper collection and processing strategies - by leading everyone through a hands-on integration and scaling of modulated single-crystal data. All of these lecturers made themselves available for one-on-one interactions with the workshop participants throughout the meeting.

The formal instruction periods of the workshop were supplemented with a number of social activities to promote networking among the participants. Each day started with a continental breakfast in the lecture hall, where everyone could mingle and discuss science with the other attendees. These discussions continued during the coffee breaks, as well as the three lunches and two dinners that were provided to the attendees. The UCSD crystallography lab, known as *Diffractopia*, was open before, during and after the workshop, and several people brought challenging crystals from their home labs to run on one of the nine state-of-the art, custom-built diffractometers in the UCSD facility. Tours of other famous UCSD landmarks, including the Geisel Library and the Fallen Star House were offered, as was a sunset hike through the Scripps Coastal Reserve near campus. No matter what their experience level and research interests were, everyone who came to this workshop learned something new and left a better scientist.

Original article: https://www.iucr.org/news/newsletter/etc/articles?issue=142706&result_138339_result_page=26

MEETING REPORT

ICTP Workshop on Crystal Structure Prediction

Artem R. OganovSandro Scandolo



Thanks to enormous progress in computing power and algorithm development, we are now closer to being able to predict the crystal structure of any material from the simple knowledge of its composition. This is the first necessary step for predicting *in silico* the property of a material and planning modifications that could improve these properties. A critical discussion of the algorithms developed in the last few years for the *in silico* prediction of crystal structures was the main theme of a workshop that took place at the Abdus Salam International Centre for Theoretical Physics (ICTP) in Trieste, Italy, from 14 to 18 January 2019. The event, titled “Workshop on Crystal Structure Prediction: Exploring the Mendeleev Table as a Palette to Design New Materials”, focused in particular on approaches based on molecular modelling and was an opportunity to celebrate 2019 as the International Year of the Periodic Table, as crystal structure prediction is rooted in a deep knowledge of the properties of the atoms, and, in turn, numerous discoveries made with the help of crystal structure prediction reveal new (often completely unexpected) sides to the behavior of the atoms.

The workshop was directed by A. Laio (Trieste), G. Desiraju (Bangalore) and the authors of this report. It was divided into two parts: the first three days were dedicated to an in-depth and critical discussion of the methods with talks given by world experts in the field. The last two days were devoted to “hands-on” computer labs where the younger participants

were given the opportunity to learn how to use the most advanced codes for crystal structure prediction, including “Universal Structure Predictor: Evolutionary Xtallography” (USPEX) and “*Ab initio* Random Structure Searching” (AIRSS).

Invited talks were given during the advanced part of the workshop by Z. Allahyari (Moscow), F. Baletto (London), V. Deringer (Cambridge), L. Ghiringhelli (Berlin), S. Goedecker (Basel), O. Isayev (Chapel Hill), E. Kucukbenli (Trieste), A. Kvashnin (Moscow), R. Martonak (Bratislava), L. Monacelli (Rome), V. Naden Robinson (Trieste), A. R. Oganov (Moscow), P. Piaggi (Lausanne), C. J. Pickard (Cambridge), A. M. Saitta (Paris), G. Schusteritsch (Cambridge), G. Tribello (Belfast), P. Villars (MPDS Co.) and Q. Zhu (Las Vegas).

The presentations highlighted methodological aspects as well as recent applications of the different methods, especially methods based on evolutionary algorithms such as USPEX (talks by Oganov, Allahyari, Kvashnin and Zhu), methods based on random sampling such as AIRSS (talks by Pickard and Schusteritsch), enhanced molecular-dynamics methods such as “metadynamics” (talks by Martonak and Piaggi), and basin-hopping methods (talk by Goedecker). Data-mining and data-based approaches were discussed by Villars and Ghiringhelli. The relevance of machine-learning methods, especially neural networks, was emphasized by many speakers, and especially by Isayev, Deringer and Kucukbenli. The hands-on sessions were led by Kucukbenli (on “Quantum-Espresso”), Allahyari (on “USPEX”) and Schusteritsch (on “AIRSS”). M. Ferri, S. Laporte and Y. Shaidu, PhD students at the International School for Advanced Studies (SISSA), provided supplementary support to the students.

Mike Glazer (Oxford), former Vice-President of the IUCr, gave a colloquium titled “Crystallography: Then, Now, and …..?”. The colloquium took place in the main lecture hall of the ICTP and was open to the entire ICTP scientific community. It was an opportunity to review the history of crystallography and highlight the important contributions given by the field to science and society.

Of the 78 participants, 23 gave lectures and 55 younger attendees presented posters and attended the hands-on tutorials. In line with the mission of the ICTP to be a global hub for science with a special regard for the developing world, participants came from 25 different countries including Cameroon, Iran, Nigeria, Congo, Argentina, Iran, Colombia and India. The workshop was co-sponsored by the European network “Psi-k”.

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Original article: https://www.iucr.org/news/newsletter/etc/articles?issue=142706&result_138339_result_page=27

MEETING REPORT

SEACOAST 2019: a new crystallographic workshop in Southeast Asia

Ruslan SanishviliRonan Keegan, Garib MurshudovLeela Ruckthong



Participants and organizers of the SEACOAST 2019 workshop.

With the robustness of the method and the highly successful automation of almost all of its steps, macromolecular crystallography is featured less prominently in a typical university curriculum. As a consequence, workshops dedicated to more systematic training in both the theory and the practice are shouldering a more and more important role in crystallographic education. The Collaborative Computational Project number 4 (CCP4) has a rich tradition of holding such workshops around the world, along with other training courses arranged by other organizations. There are now regularly organized workshops in Europe, USA, South America and Asia. One region that is much less represented in this aspect is Southeast Asia.

The Workshop

To address this issue, King Mongkut's University of Technology Thonburi (KMUTT) in Bangkok, Thailand, hosted an inaugural workshop entitled "SouthEast Asian Crystallographic Overview And Systematic Training" (SEACOAST). The workshop was held from 21 to 26 January 2019 and was focused on fundamentals of crystallography and modern crystallographic computational tools. It was organized by Ruslan Sanishvili (Nukri) from Argonne National Laboratory, USA; Ronan Keegan, CCP4, STFC Rutherford Appleton Laboratory, UK; and Garib Murshudov MRC LMB, UK; with Leela Ruckthong of KMUTT

taking the lead in all aspects of local organization. All steps of macromolecular crystallography, from cloning and protein purification to structure refinement and bioinformatics, were addressed by 14 local and international speakers: Terese Bergfors, Uppsala University, Sweden; Ronan Keegan, CCP4, Harwell, UK; Eugene Krissinel, CCP4, Harwell, UK; Andrey Lebedev, CCP4, Harwell, UK; Andrew Leslie, MRC LMB, Cambridge, UK; Bernhard Lohkamp, Karolinska Institutet, Sweden; Garib Murshudov, MRC LMB, Cambridge, UK; Nuttawan Pramanpol, SLRI, Thailand; Leela Ruckthong, KMUTT, Thailand; Marasri Ruengjitchatchawalya, KMUTT, Thailand; Ruslan Sanishvili, APS, Argonne National Laboratory, USA; Tom Terwilliger, Los Alamos National Laboratory, USA; Andrea Thorn, University of Wuerzburg, Germany; and Clemens Vonrhein, Global Phasing Ltd, Cambridge, UK.

The daily schedule was made up of lectures in the morning to introduce the theory and concepts of macromolecular crystallography, followed by tutorials on software programs and hands-on problem-solving sessions where the participants worked on their own difficult data with lecturers providing expert guidance.



Garib Murshudov (left) and Andrea Thorn giving lectures.

Participation

SEACOAST 2019 was mainly intended for graduate students, postdoctoral researchers and early career scientists from academic and industrial institutions. The workshop attracted considerable interest from researchers in the Southeast Asian region and beyond. The group of 30 participants, selected from an applications pool, comprised the trainees from Thailand, Malaysia, Singapore and Japan, represented by a broad spectrum of expertise from novices to structural biologists with considerable experience, and a wide range of

scientific projects from studying chemical composition in spent grains to understanding the origins of cell evolution.

Impact

About half of the class were novices in macromolecular crystallography while the other half had reasonable experience. The content of the workshop, which comprised a theoretical foundation, tutorials and hands-on sessions, was a perfect fit for such a wide range of knowledge base. Less experienced students benefitted from in-depth lectures on theory to establish a solid foundation on which to build further learning. Researchers with problem data sets deepened their knowledge in basics and were able to resolve the technical challenges they faced in their projects.

Out of the selected 30 applicants, 14 brought their own data to work on during the problem-solving sessions. Seven new structures were solved within this group during the workshop, utilizing both experimental phasing, including S-SAD, and molecular replacement. Some of the projects benefitting from these newly solved structures included the *p*-hydroxyphenylacetate (Hpa) degradation pathway, which is important in the degradation of natural and synthetic aromatic compounds; multi-drug resistance; antimalarial drug development; anti-parasitic inhibition; and biocatalysts in a broad range of natural, synthetic and degradation processes.

Feedback

The primary purpose of SEACOAST 2019 was to promote and enhance crystallographic education in the Southeast Asian region. The workshop was successful in achieving this goal, as attested by the feedback received from the students and lecturers in private conversations and in an anonymous survey: “The course was very useful. I learned fundamentals which are not taught in regular school courses.” “I learned the importance of data collection and data processing.” “This workshop is a great opportunity for people working in the field of crystallography. It enhances our knowledge of fundamentals of the technique of crystallography.”

The same was evident in a more formalized survey where specific aspects of the workshop were ranked according to the level of satisfaction.

Future

Encouraged by the success of SEACOAST 2019, we are planning to organize a similar workshop in the second half of January 2020. While all aspects of the workshop garnered high praise, both the students and the lecturers made a number of useful suggestions and we believe incorporating these ideas will further elevate the quality of the next workshop. We are also considering adding a data collection component where the participants will acquire practical data collection skills from hands-on experiments at synchrotron beamlines.

Acknowledgements

We would like to express our gratitude to the KMUTT; Faculty of Science, KMUTT; Department of Chemistry, KMUTT; and Science and Technology Facilities Council, UK for their generous funding of the workshop, and to the Thailand Research Fund; Horiba

Scientific; Protein Society of Thailand; N K LABORATORY, (THAILAND) CO. LTD; IRPC; LAB SYSTEMS CO. LTD and T.S. Inter Lab Limited Partnership, for their generous contributions as well.

We are sincerely grateful to the former and current presidents of KMUTT, Sakarindr Bhumiratana and Suvit Sae Tia, respectively; the dean of the Faculty of Science, Thiradet Jiarasuksakun; the advisor to the president, Vanida Bhavakul; and the head of the Chemistry Department, Anawat Pinisakul for their support and encouragement, and to members of the Department of Chemistry and the Department of Mathematics for their assistance.

LR and RS are indebted to Wittawin Susutti for his help in the workshop website design and maintenance, and to the lecturers at the workshop with their selfless dedication to crystallographic education and teaching at the SEACOAST workshop.

Original article: https://www.iucr.org/news/newsletter/etc/articles?issue=142706&result_138339_result_page=28

MEETING REPORT

Gender parity in science roundtable

Michela Brunelli



Photo: ESRF/C. Argoud.

A roundtable on "Gender parity in science" was organized at the European Synchrotron Radiation Facility (ESRF) by the ESRF User Organization during the first day of the annual User Meeting (4 February 2019). This was the first time that an event on the subject had been hosted at the European Synchrotron, and the presence of about 80 participants in the Auditorium (~25% men) surpassed our expectations.

The invited Speakers and Guests were Cornelius Gross [Deputy Head, European Molecular Biology Laboratory (EMBL)-Rome], Eva Pebay-Peyroula (former Institut de Biologie Structurale Director), Christiane Alba-Simionesco (CNRS, former Laboratoire Léon Brillouin Director), Brigitte Plateau (General Administrator of Institut Polytechnique de Grenoble and "Directrice Générale de l'enseignement supérieur et de l'insertion professionnelle en Conseil des Ministres"), Jean Daillant (Soleil Synchrotron General Director) and Sine Larsen (former ESRF Director). Francesco Sette (ESRF General Director) was also present.

The aim was to debate questions such as what slows down the progression of women's careers, considering that women and men with the same qualifications often do not have access to the same career path, and can different recruitment strategies improve women's success rates in job interviews. Furthermore, what actions can institutions carry out to help break the glass ceiling and reach the needed gender balance?

Guests were asked to comment on their working conditions and to discuss if any measures were implemented in their institute to balance between private life and the professional career.

C. Gross and E. Pebay-Peyroula opened the roundtable with two 15-minute talks, and the ESRF Head of Administration presented statistics on women's presence at different scientific career levels in the Experimental Division of the ESRF, indicating the presence of a glass ceiling effect.

C. Gross, as chair of the EMBL Equality & Diversity Committee, gave a talk on “Perspectives on Gender Balance at EMBL” that, along with statistics, illustrated how EMBL is trying to improve its recruitment and employment policies. Among its actions in this direction, it supports proactive solicitations, a dual-career pilot project, and childcare and on-site nursing rooms. More generally, it tries to promote diversity among role models (speakers and mentors) and resist stereotypes in our general culture. EMBL’s results in terms of recruitment were impressive.

E. Pebay-Peyroula’s contribution gave a historical perspective by showing the evolution of the role of women in science since Rosalind Franklin. She commented on women's situation (stereotypes, judgments, differences) in family, school and higher education from the 1930s and 40s to now. As Director and evaluation panel member, she was able to give a personal view of evaluating and self-valuating excellence in science, questioning the benefits of “good examples” and/or “too good examples” with the provocative query “Is Marie Curie a good example?” for women in science.

Guests completed the discussion with personal testimonials, examples of actions in their institutes and an update on current French regulations.

The roundtable was animated by Giovanna Fragneto and Nedjma Bendiab from the “Parité-Science” Association, a French association that strives for parity in scientific and technical professions, and generated a rich debate within the public. The consensus was that gender parity in science could be achieved with proactive actions of the administration of our institutes, together with national policy and a personal stand against stereotypes.

Original article: https://www.iucr.org/news/newsletter/etc/articles?issue=142706&result_138339_result_page=29

MEETING REPORT

First International Conference on "Crystal Engineering: From Molecule to Crystal"

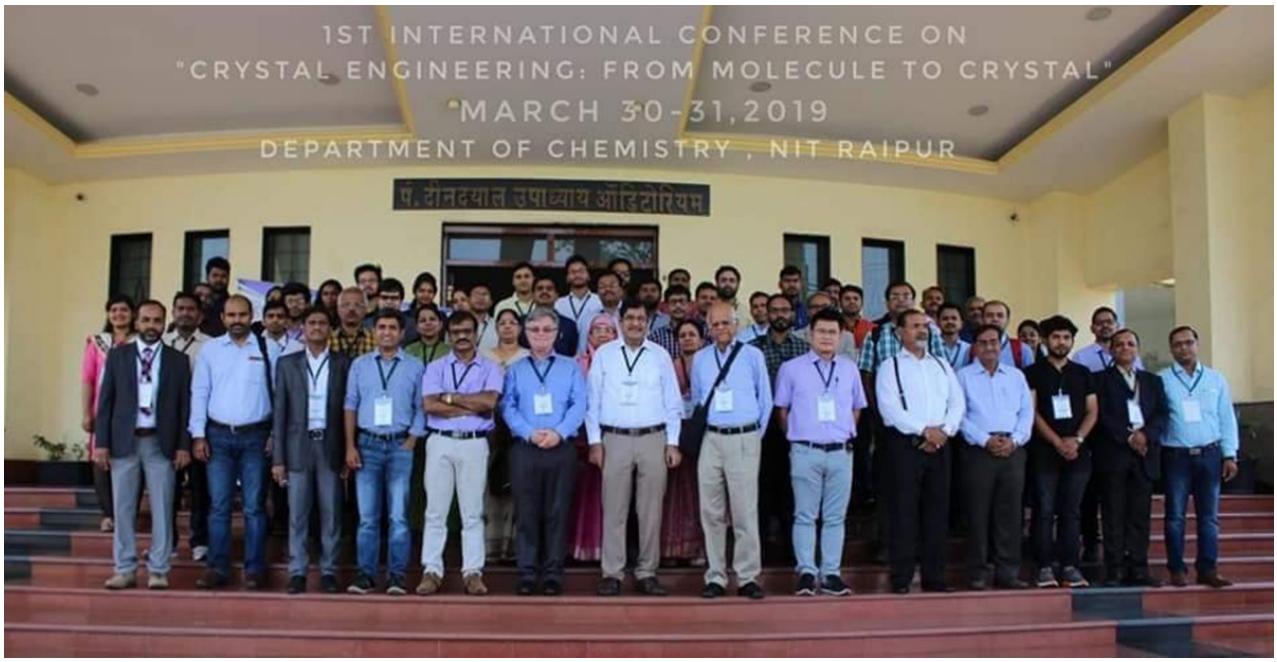


The First International Conference on "Crystal Engineering: From Molecule to Crystal" (CE:FMC2019) was held from 30 to 31 March 2019 in Raipur. Raipur is the capital city of Chhattisgarh state in central India. The conference was organized by the Department of Chemistry at the National Institute of Technology (NIT) Raipur, and was attended by 70 participants from India and neighboring countries. The two-day format included two Plenary lectures (1 hour each), four Keynote lectures (40 minutes each) and nine invited talks (30 minutes each). In addition, there were 10 oral (20 minutes each) and 20 flash oral (2 minutes each) contributions selected by the Scientific Committee from the submitted abstracts. The poster session enabled about 25 participants to share their work in this exciting meeting for the crystal engineering community.

The Indian Crystallographic Association (ICA) supported the conference by providing a fund of INR 25,000 for conference expenditure and two best poster and two best flash oral awards. The Science and Engineering Research Board, Department of Science and Technology (SERB-DST), India, supported the conference by providing a fund of INR 125,000 for travel/accommodation of Senior and Young Scientists and pre-conference printing. The invitation to attend the conference as Plenary lecturers was kindly accepted by Gautam R. Desiraju (IUCr Past President) and Edward R. T. Tiekink (Sunway University, Malaysia). The CE:FMC2019 also had the pleasure of hosting four other eminent scientists as Keynote speakers, Kumar Biradha (Associate Editor, *Crystal Growth & Design*; IIT Kharagpur, India), C. Malla Reddy (IISER Kolkata, India), Kittipong Chainok (Thammasat

University, Thailand) and R. Vaidhyanathan (IISER Pune, India), and 10 young scientists as invited speakers.

In general, the conference covered a wide range of topics: single-crystal and powder diffraction, chemical crystallography, crystal engineering, charge density, quantum-chemical and database studies, and materials science. The event passed in an informal and friendly atmosphere with stimulating discussions during the sessions as well as in the coffee breaks, lunch and conference dinner. We hope that the conference helped our young colleagues to get better acquainted with the possibilities of contemporary crystallographic research and to recognize appropriate methods for further improvement of their work. The second conference in the series, CE:FMC2020, is scheduled to be held at Visvesvaraya National Institute of Technology Nagpur, India. The General Assembly of CE:FMC2019 evaluated the conference as very successful, and the generous support from the NIT Raipur, ICA, SERB-DST, IR TECH and TCI was gratefully acknowledged.

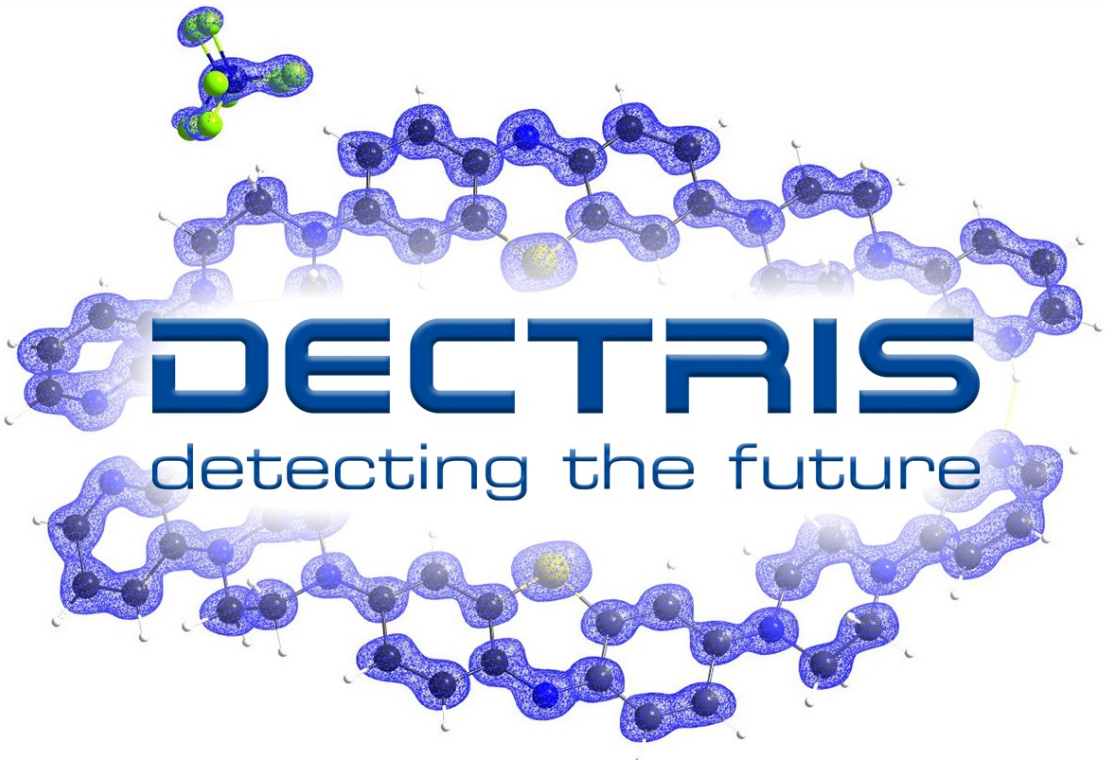


Original article: https://www.iucr.org/news/newsletter/etc/articles?issue=142706&result_138339_result_page=30

ADVERTISING FEATURE

Electron diffraction of submicron-sized 3D crystals

Andreas FörsterSacha De Carlo



In the past six months we have witnessed a surge of interest in electron diffraction. An increasing number of papers have described the use of this technique to solve crystal structures from samples that were previously thought beyond the reach of X-ray diffraction, with an ease and speed that made commentators wonder why this hadn't been done before. Here, we are going to review recent developments in the field, address outstanding questions and give an outlook for the near future.

The structural information that synthetic chemists and the pharmaceutical industry need is often extracted from crystalline material using X-rays. Single-crystal X-ray diffraction is a mature technique that gives the most detailed structural information. The bottleneck lies in the sample itself: the steps required to obtain a crystal suitable for data collection are hard to control. A crystal must be well ordered and sufficiently large to give useful diffraction spots. Obtaining such a single crystal is not trivial and largely depends on the behavior of the compound(s) under study, in particular their homogeneity and flexibility. This is a particular problem for macromolecular samples, but even smaller molecules do not always crystallize sufficiently well.

In the absence of diffraction-quality crystals, powder X-ray diffraction and nuclear magnetic resonance spectroscopy provide alternative routes to atomic structures, but their power pales next to that of single-crystal X-ray diffraction. The recent interest in

microcrystal electron diffraction (MicroED) is based on the promise of atomic structures from powders in a straightforward manner.

MicroED exploits two key features of electrons: their short wavelength and their strong interaction with matter. In a typical transmission electron microscope (TEM), electrons are accelerated to energies of 200 or 300 keV, giving wavelengths of 0.025 and 0.020 Å, respectively. Atomic resolution is thus within the reach of all modern TEMs. The strong interaction of electrons with matter means that much less diffracting material is required to obtain strong reflections.

The physics of electrons is nothing new. The recent excitement around MicroED stems from the fact that it is now technically possible to collect accurate diffraction data from microcrystallites with dimensions around 100 to 500 nm and to process and analyze these data to obtain atomic structures. Materials that crystallographers would dismissively qualify as powders frequently turn out to be microcrystalline, with crystallites of dimensions of the order of a few dozen to a few hundred nanometres. Although they might be invisible to the naked eye, these microcrystals are excellent targets for MicroED.

MicroED can be done using TEMs, which are in common use in laboratories (see Figure 1). In these instruments, hundreds of crystals can be deposited and screened on one 3 mm disk used as a support (the “grid”), a process that can be automated to some extent. Once a good crystal is found, data collection takes only a few seconds when using hybrid pixel detectors for direct electron detection in shutterless mode (Smeets *et al.*, 2018; Heidler *et al.*, 2019). If throughput is not an issue, the use of standard charge-coupled devices can provide good results within less than 15 min per compound, as illustrated in a recent paper by the Gonen group (Jones *et al.*, 2018), which has been successfully using MicroED on protein nanocrystals since 2013 (Shi *et al.*, 2013).

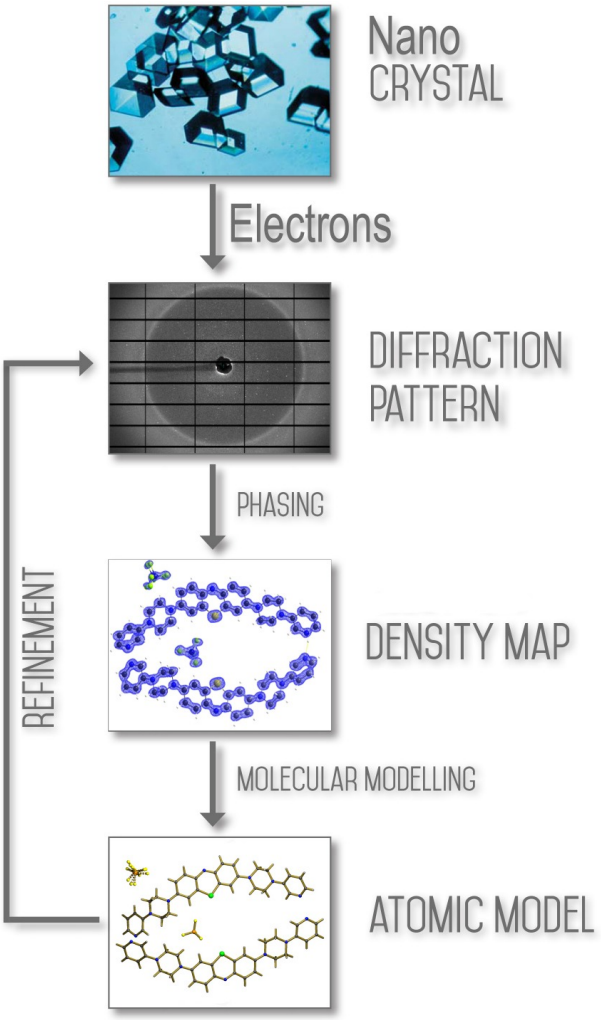


Figure 1. The MicroED workflow. Tiny crystals, less than half a micron in thickness, can be found in imaging mode and then exposed to electrons in diffraction mode using the rotation method. After indexing and integration, phases are calculated by direct methods or molecular replacement.

Recent MicroED highlights include the structure of a previously uncharacterized organic compound, a new methylene blue derivative, that was determined in a semi-automated and cost-efficient experiment, similarly to what is routinely achieved in modern structural chemistry labs equipped with X-ray diffractometers (Grüne *et al.*, 2018). Grüne and colleagues also demonstrated the potential of MicroED as an important tool in the courtroom. When it comes to identifying polymorphs, crystal structures determined with MicroED can provide clearer answers than those determined with powder X-ray diffraction (Figure 2). At the 31st Meeting of the European Crystallographic Association in Oviedo, Spain, in 2018, Joel Bernstein (Ben-Gurion University, Beer-Sheva, Israel) stated that "the existence of multiple crystal forms such as polymorphs, solvates, hydrates *etc.*, is playing an increasingly important role in establishing and protecting intellectual property rights in the pharmaceutical industry".

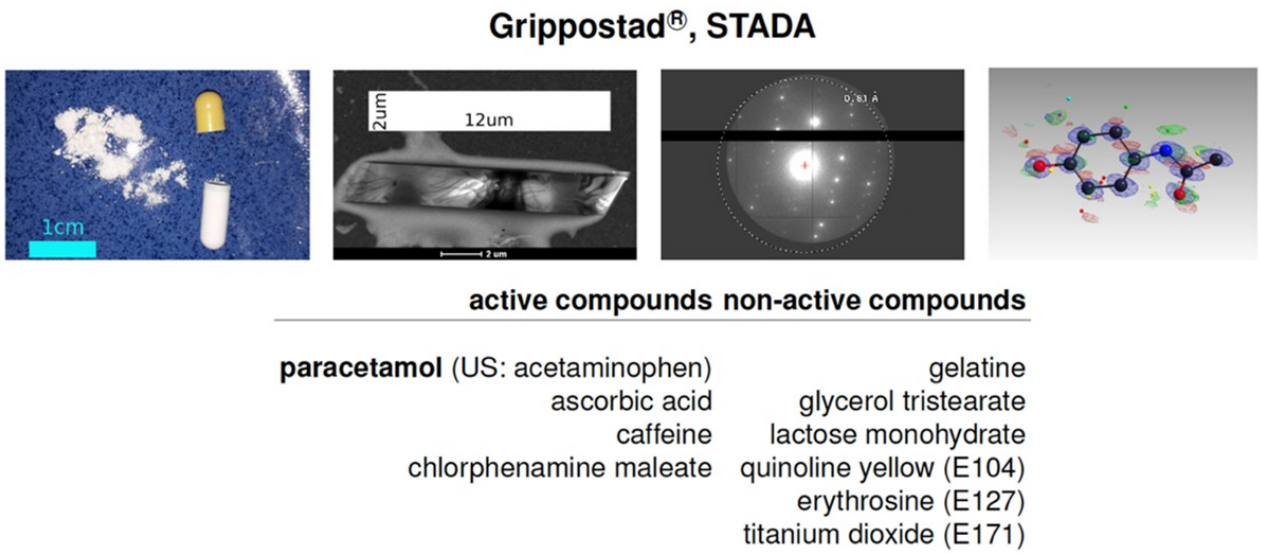


Figure 2. The process of applying MicroED to a pharmaceutical compound. The active ingredient (paracetamol) in the commercially available common cold remedy Grippostad® was analyzed from powder taken directly from the drug capsule. The process of determining the structure at atomic resolution took less than 30 min from sample preparation to visualizing the molecule (Grüne *et al.*, 2018).

A major problem of MicroED data is poor statistics. *R* values are much higher than in X-ray crystallography. The reasons for this include hardware optimized for imaging, algorithms written for X-ray diffraction data, poor scaling, and background caused by inelastic and multiple scattering events. Despite the poor statistics, atom identities can be distinguished with MicroED data (Palatinus *et al.*, 2017), as long as the resolution is high enough (see Figure 3). MicroED has been used to solve the structure of more than 40 known proteins and new oligopeptides (Nannenga & Gonen, 2019) as well as novel proteins (see Figure 4 and Xu *et al.*, 2019). There tend to be no differences between structures determined by MicroED and those determined by X-ray crystallographic techniques.

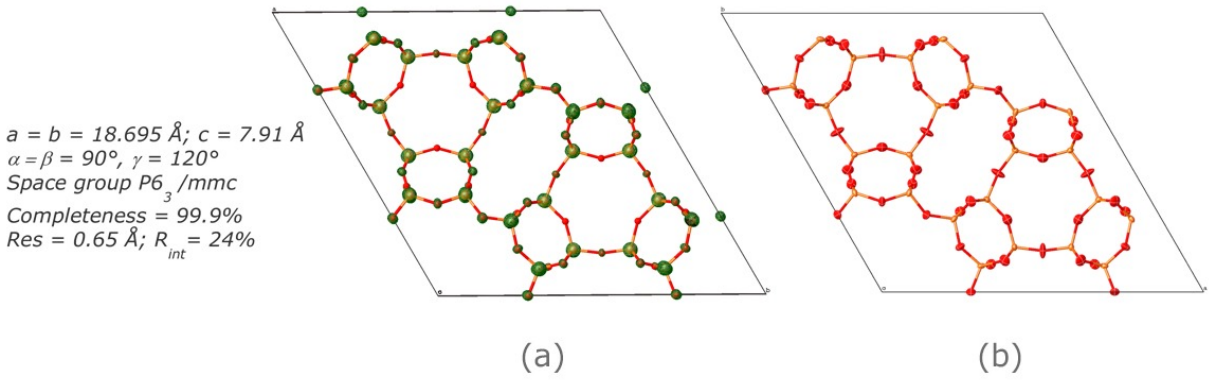


Figure 3. Omega-form zeolite of the MAZ framework (http://europe.iza-structure.org/IZA-SC/framework.php?STC=MAZ); (a) MAZ structure with Coulomb potential densities superimposed in green, (b) corresponding atomic model (oxygen red, silicon orange). We acknowledge Amy Knorpp (ETH Zürich, Switzerland) for the sample and Julian Wennmacher (Paul Scherrer Institute, Villigen, Switzerland) for the processed data.

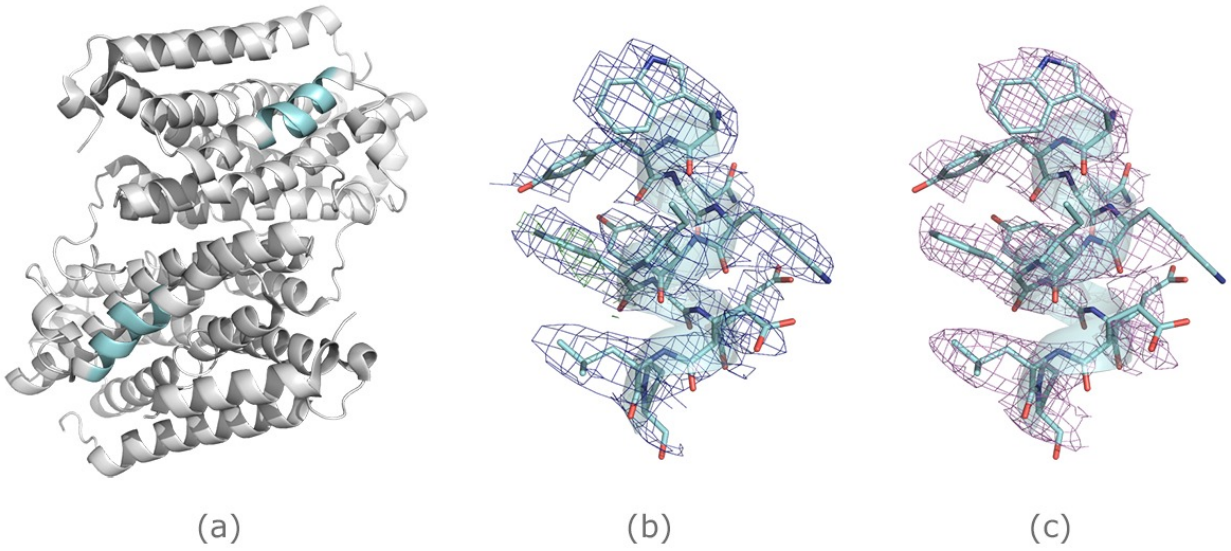


Figure 4. (a) Overall structure of the dimeric assembly of SaR2lox (which is the physiological oligomerization state of the protein in solution). (b) Electrostatic scattering potential maps $2F_o$-F_c (blue, contoured at 1 sigma) and F_o-F_c (greed/red, contoured at 3 sigma) shown for residues 142 to 152 (Trp142 - Pro152, carbon cyan, oxygen red, nitrogen blue). (c) Simulated annealing composite omit map (magenta, contoured at 1 sigma) shown for the same residues. We acknowledge Max Clabbers (Stockholm University, Sweden) for providing us with this figure, modified from Clabbers *et al.* (2019).

To improve the quality of the data that can be obtained with MicroED, a specifically designed tool with a high degree of automation and integration is required. This would also be indispensable for the high-throughput workflows in structural chemistry and pharmaceutical laboratories. Grüne and collaborators have suggested design guidelines for such an electron diffractometer (Heidler *et al.*, 2019; see Table 1). Some of these features are already available in certain TEMs that can thus be adapted for MicroED. For a commercially successful electron diffractometer, these elements need to be individually optimized and matched to provide the necessary speed and data quality for MicroED and an optimal user experience.

Two of the improvements identified by Grüne and co-workers, parallel illumination (also called Köhler illumination, see Benner & Probst, 1994) and in-column energy filters, were available as standard configuration in medium-range TEMs manufactured by ZEISS. Since ZEISS stopped TEM production in 2013, these configurations have been available only in costly high-end systems, even though this configuration would be desirable for a cost-effective electron diffractometer. Parallel illumination ensures that only a small portion of the sample is illuminated when imaged, which avoids overall pre-irradiation of surrounding unexplored areas. It also avoids image distortions while keeping the beam incidence perpendicular at every point of the specimen, and provides a very useful simple switchover from TEM to scanning TEM mode (useful for observing tiny crystals at low magnification).

Table 1. List of desirable improvements for a dedicated electron diffractometer

Item	**Benefit**
Parallel illumination	More coherent illumination at the specimen. Easy switch from imaging to diffraction and *vice versa* while minimizing lens hysteresis.

Item	Benefit
High-precision goniometer	Higher precision at higher angular speed improves the throughput for single-crystal data collection.
Embedded hardware	Seamless integration of hardware and software enables synchronizing of the goniometer motion and triggering of the detector while the experimental parameters required for data processing are transferred as metadata.
Energy filter	The removal of inelastically scattered electrons reduces background noise in the diffraction pattern.
Noise-free fast detector	An energy-discriminating, single-quantum counting detector with very high dynamic range, withstanding the direct electron beam and with kilohertz readout for fine slicing.

Energy filters remove inelastically scattered electrons, which improves the signal-to-noise ratio (Yonekura *et al.*, 2002; 2019). The energy filter also plays a role in the sample selection, in the sense that sample thickness can be measured directly and quantitatively. In addition, as a thin planar crystal is rotated along its plane axis, the electron path through it increases and with it the inelastic scattering cross-section. Use of an energy filter would mitigate this effect and lead to better data. Thicker crystals could in principle be analyzed with higher-energy electrons, but this would increase the overall cost of the dedicated electron diffractometer. An acceleration voltage of 120 keV is sufficient for good MicroED data (*cf.* the work of Gemmi's group in Pisa, Italy; Lanza *et al.*, 2019).

The detector is another important element in a dedicated electron diffractometer. With a readout speed greater than 2000 frames s^{-1} and no dead time, hybrid pixel detectors would synchronize very well with an optimized precision goniometer, similar to those used in X-ray crystallography, and allow for high-throughput operation.

The dynamic range of the detector is important to accurately record reflections with vastly different intensity values (four to six orders of magnitude). This requires a dynamic range of at least 20 bits, which is provided only by electron-counting devices of the hybrid pixel type, such as Medipix-based detectors and PILATUS and EIGER (Brönnimann & Trüb, 2019), which are widely used in high-energy physics and X-ray crystallography.

Another aspect of a successful electron diffractometer is tightly integrated software for instrument control and data analysis. Here, great progress has already been made by a few groups. For example, the SerialED software suite (Smeets *et al.*, 2018) can control both the beam and the detector to successfully perform serial electron crystallography at a staggering rate of 3500 crystals per hour. The software is open source, and the lab also shared a suite for offline data processing.

Once the technical aspects of MicroED have been addressed, MicroED will become increasingly useful for structural chemistry and structure-based drug design. It is likely to fill the gap between single-crystal and powder X-ray diffraction, and make structure determination faster and easier. Will it replace X-ray diffraction? The two techniques have complementarities that will not disappear any time soon. X-ray crystallographic techniques provide data of the highest accuracy for crystals in the micrometre range. If crystals cannot be grown to this size, MicroED can be used to determine their structures.

The time when electron diffraction will match X-ray diffraction as a method for structural chemistry and pharmaceutical development is getting closer and closer!

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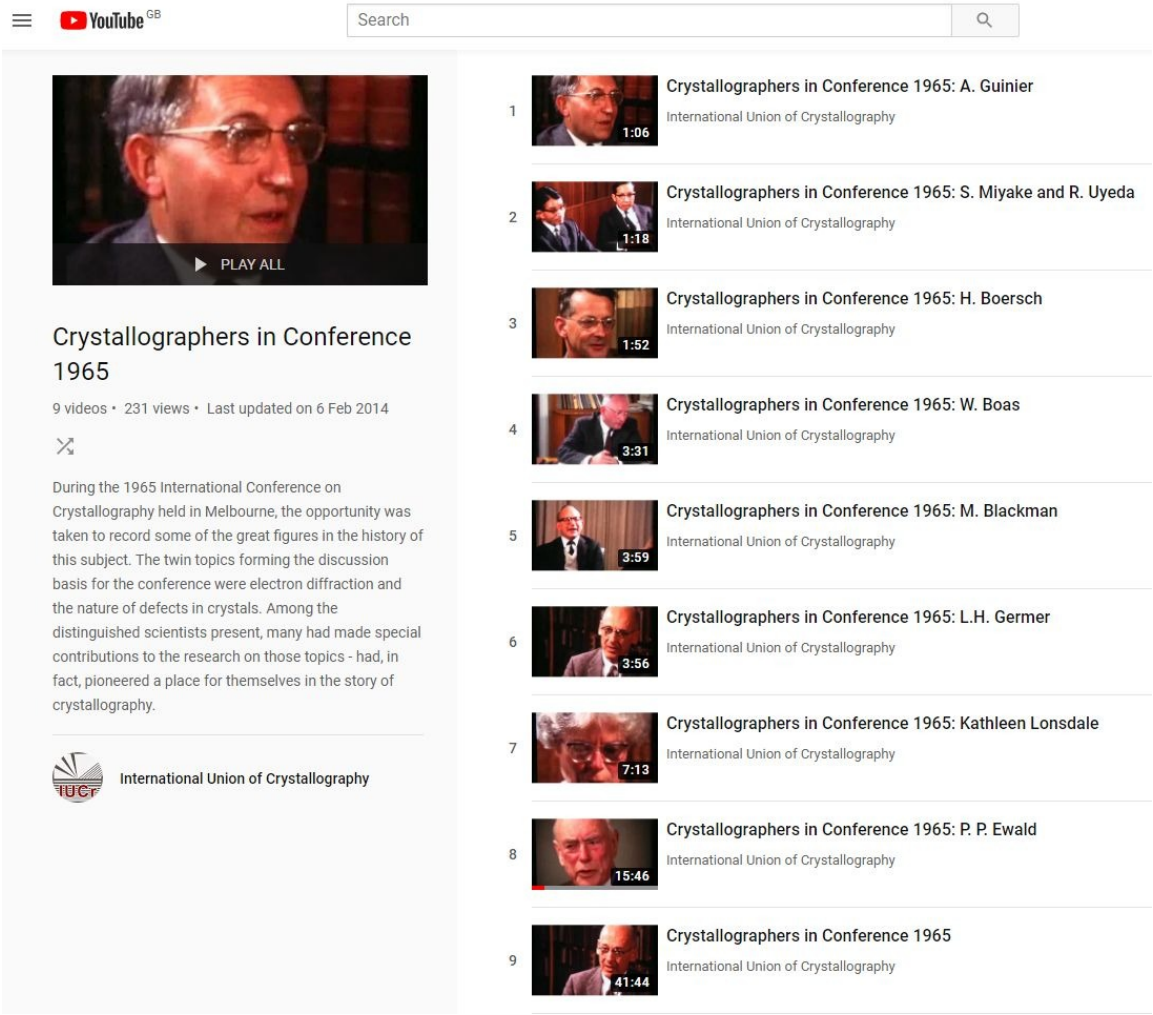
Conferencing down under

Andrew Johnson



Among the materials science advances during the 1960s, crystallography played a vital role in the explanation of non-stoichiometry in oxides by means of crystallographic shear; at the same time, resolution improvements in transmission electron microscopy (TEM) allowed their imaging. In addition, the properties of dislocations were being elucidated by TEM imaging and diffraction and advances in the theory of multiple scattering of electrons were giving rise to improved understanding of imaging and diffraction results. It was therefore decided to hold a conference in Melbourne, Australia, so that workers in these different fields could better communicate. Such was the interest in this major interdisciplinary conference that a wide variety of leading scientists from around the world attended, and many stayed on to attend a subsequent satellite workshop on the study of crystal defects by diffraction methods.

An account of the conference was published in *Acta Crystallographica* (1966), **21**, 455-457, and gives a flavour of the significance of the meeting. The CSIRO Film Unit took advantage of the occasion to film a number of interviews with many of the distinguished participants, who included many of the founding figures of modern crystallography and electron diffraction. These recordings are available through the IUCr YouTube channel and are of great historic interest.



Interviews with distinguished crystallographers attending the 1965 Conference on Crystallography in Melbourne.

The satellite meeting took place at the Mayer Chalet at Warburton, near Melbourne, from 23 to 25 August 1965, and a group photograph showing the participants is in the IUCr photographic archive. We have been able to identify a number of the participants as shown in the figures below, thanks to the help of Jimpei Harada (both very fortunate as young scientists to meet such a distinguished group of crystallographers), but we would be very interested to identify more of the participants, or to hear any personal recollections of that workshop or the Melbourne Conference. If you are able to help, please send information *via* the gallery link above or by email to support@iucr.org.



Annotated extract of the group photograph of participants of the Warburton school on crystal defects.

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OBITUARY

Barbara Wharton Low (1920-2019)

Jenny P. Glusker



Barbara Wharton Low, Emeritus Professor at Columbia University, New York, USA, passed away on 10 January 2019, aged 98 years. She was an X-ray crystallographer who played an active role in the determination, with Dorothy Hodgkin in 1949, of the previously contested chemical formula of the important antibiotic penicillin. She then went to Caltech and worked in the laboratory of the X-ray crystallographers Linus Pauling and Robert Corey. There, in 1952, she reported her discovery of an additional manner of polypeptide folding in proteins to that of the α-helix; she named it the 'π-helix.' Since that time she was an Assistant Professor of Physical Chemistry at Harvard University in Boston where she was among the first to introduce X-ray diffraction studies of crystalline proteins into laboratories in the United States. Then, in 1956, she moved to Columbia University of Physicians and Surgeons in New York where she continued studies of protein structure, becoming a full Professor in 1966. She remained there until her retirement in 1990. A much admired teacher and mentor, she continued to lecture there for most of the rest of her life.

Barbara was born in Lancaster, England, on 23 March 1920. She was a bright student, interested in science, and studied chemistry at Somerville College, Oxford University, with Dorothy Crowfoot Hodgkin as her tutor and mentor. Barbara obtained a BA degree in chemistry in 1946 and stayed on for graduate research in Dorothy Hodgkin's laboratory, obtaining a DPhil degree from Oxford University in 1948.

Barbara did her undergraduate and graduate experimental studies with Dorothy Hodgkin on penicillin. The antibiotic activity of penicillin had originally been discovered by Alexander Fleming in 1928, and was being studied extensively in England and the United States. It had been first used on patients in 1943 and had served well in eliminating infections in many patients. In Oxford, penicillin research was led by Howard Florey, Norman Heatley and Ernst Boris Chain. Ernst Chain worked on its purification and managed to crystallize its sodium salt. He gave Dorothy some crystals, and those were the ones that Barbara worked on.

The chemical formula of penicillin, uncertain at that time, was eventually found as the result of collaborations between Dorothy Hodgkin and Barbara Low at Oxford University with Charles William Bunn and Anne Turner-Jones at Imperial Chemical Industries (its Alkali Division in Winnington, Northwich). However, these were the early days of structure determination by X-ray diffraction of crystals, and the work was difficult and hard because there were so many experimental data to deal with and computational equipment was just beginning to be used for such types of scientific research. Techniques for interpreting the diffraction data in terms of molecular structure were being worked out from day to day. The use of Beevers–Lipson strips, which provided a method for calculating electron-density maps, took much time, whereas this has become much quicker since computer programs have become available. Penicillin was one of the largest structures studied at that time. This work in Oxford was described in more detail by Georgina Ferry in her book *Dorothy Hodgkin: A Life*, published by Grant Books in 1998.

The resulting structure of penicillin that was determined in Oxford, however, was highly significant because the chemical formula for penicillin had not been known before the X-ray diffraction studies were completed. The crystal structure showed that penicillin contained a four-membered β-lactam ring fused to a five-membered ring – an overall structure that is very active chemically (and favored by Howard Florey in Oxford and by Professor Woodward at Harvard). This finding of a β-lactam ring was appropriate for its biochemical action of interference with the three-dimensional structure within bacterial cell walls. The Oxford Professor of Chemistry, Sir Robert Robinson, was convinced, however, that penicillin had a different formula – that of a less-active thiazolidine-oxazolone structure (two five-membered rings connected by a single bond). It was therefore suggested that maybe the X-rays used in the diffraction experiment had caused the conversion of penicillin from an oxazolone to a β-lactam structure. To satisfy the questioning chemists, Dorothy and Barbara were able to show that their crystals of penicillin after exposure to X-rays (and proven to have the β-lactam structure) were the biologically active form of penicillin; they did not start with a thiazolidine structure that had been damaged (and therefore converted to β-lactam structure) by X-ray exposure during diffraction studies. The chemical community then accepted the formula that Dorothy and Barbara had found.

This crystal structure was published in 1949 (70 years ago) in an article entitled 'The X-ray Crystallographic Investigation of the Structure of Penicillin' by D. Crowfoot (Hodgkin), C. W. Bunn, B. W. Rogers-Low and A. Turner-Jones, in a book entitled *The Chemistry of Penicillin*, by H. T. Clarke, J. R. Johnson and R. Robinson (Princeton University Press). The Nobel Prize in Chemistry 1964 was awarded to Dorothy Crowfoot Hodgkin 'for her determinations by X-ray techniques of the structures of important biochemical substances', and penicillin was

one of these compounds. The determination of the chemical formula in World War II was a very significant event, leading to the possible chemical synthesis of the compound and the design of more active derivatives, thereby saving the lives of many wounded soldiers.

Barbara then came to the United States and continued structural studies in the laboratory of Linus Pauling and Robert Corey at Caltech in Pasadena, California. She became interested in current structural studies of helical folding in proteins by these professors, and what it indicated about protein structure. Her primary studies led to her finding of the π-helix in which each N–H group forms a hydrogen bond with a C=O group of an amino acid five residues earlier in the polypeptide chain. This helix, which she described in 1952 while at Harvard, was different from the α-helix that Linus, Robert and Herman Branson had proposed as a prominent form of polypeptide folding in the spring of 1951. Her graduate student, Richard B. Baybutt, had modeled the π-helix by accident while he was building an α-helix, and Barbara had recognized the importance of this alternate hydrogen-bonded arrangement. Whereas a π-helix is much less common in proteins than an α-helix, it has been found that the addition or deletion of a single amino acid in a protein can be sufficient to interconvert α-helices and π-helices. This relationship may be important in evolutionary changes in protein function. When the π-helix is found in certain proteins it appears to facilitate their action, for example, by helping bind a metal ion that enhances the activity of the protein (as in lipogenase) or forming a hump in an α-helix. Barbara described this π-helix at the Pasadena Conference on the Structure of Proteins in 1953.

Barbara moved to Harvard (1948-1956) and became an Assistant Professor of Physical Chemistry where she studied crystalline proteins. She had married Metchie J. Budka in 1950 and had become a US citizen. She then moved to the College of Physicians and Surgeons, Columbia University, New York in 1956, where she continued studies of protein structure. She taught other crystallographers many details of the optimum experimental conditions of proteins in structural work, such as how or whether to lower the temperature. Initially she studied crystals of insulin and proinsulin, presumably as a follow-up of her work with Hodgkin. Her main work now involved neurotoxic proteins obtained in the very poisonous venom of sea snakes from the Pacific Ocean. The venom some produce is known to bind to the acetylcholine receptor and inhibit it. Her structural work on the three-dimensional structure of the neurotoxin sea-snake venom, erabutoxin, shows that it forms a three-finger-like structure that provides a concave surface to which the acetylcholine receptor can bind with disastrous consequences to anyone receiving a bite from the sea snake. This work has led to investigations by several scientists on the nature of the atomic interactions that lead to the inhibition of the acetylcholine receptor.

Barbara Low, as a researcher and teacher, inspiring many students, has made several important discoveries in biochemistry and medicine. She was appreciated for her careful research in the early days when X-ray diffraction studies were difficult and her later investigations on larger molecules have contributed to the greater efficiency of structure determination and our understanding of chemistry and physics today.

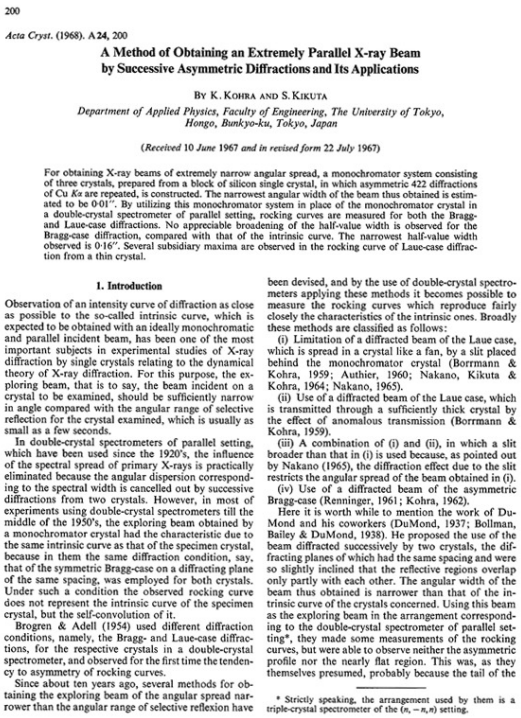
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OBITUARY

A tribute to Kazutake Kohra (1921-2019)

Yoshiyuki Amemiya





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Acta Cryst. (1968). A24, 200

A Method of Obtaining an Extremely Parallel X-ray Beam by Successive Asymmetric Diffractions and Its Applications

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(*Received* 10 *June* 1967 *and in revised form* 22 *July* 1967)

For obtaining X-ray beams of extremely narrow angular spread, a monochromator system consisting of three crystals, prepared from a block of silicon single crystal, in which asymmetric 422 diffractions of Cu $K\alpha$ are repeated, is constructed. The narrowest angular width of the beam thus obtained is estimated to be 0·01″. By utilizing this monochromator system in place of the monochromator crystal in a double-crystal spectrometer of parallel setting, rocking curves are measured for both the Bragg- and Laue-case diffractions. No appreciable broadening of the half-value width is observed for the Bragg-case diffraction, compared with that of the intrinsic curve. The narrowest half-value width observed is 0·16″. Several subsidiary maxima are observed in the rocking curve of Laue-case diffraction from a thin crystal.

1. Introduction

Observation of an intensity curve of diffraction as close as possible to the so-called intrinsic curve, which is expected to be obtained with an ideally monochromatic and parallel incident beam, has been one of the most important subjects in experimental studies of X-ray diffraction by single crystals relating to the dynamical theory of X-ray diffraction. For this purpose, the exploring beam, that is to say, the beam incident on a crystal to be examined, should be sufficiently narrow in angle compared with the angular range of selective reflection for the crystal examined, which is usually as small as a few seconds.

In double-crystal spectrometers of parallel setting, which have been used since the 1920's, the influence of the spectral spread of primary X-rays is practically eliminated because the angular dispersion corresponding to the spectral width is cancelled out by successive diffractions from two crystals. However, in most of experiments using double-crystal spectrometers till the middle of the 1950's, the exploring beam obtained by a monochromator crystal had the characteristic due to the same intrinsic curve as that of the specimen crystal, because in them the same diffraction condition, say, that of the symmetric Bragg-case on a diffracting plane of the same spacing, was employed for both crystals. Under such a condition the observed rocking curve does not represent the intrinsic curve of the specimen crystal, but the self-convolution of it.

Brogren & Adell (1954) used different diffraction conditions, namely, the Bragg- and Laue-case diffractions, for the respective crystals in a double-crystal spectrometer, and observed for the first time the tendency to asymmetry of rocking curves.

Since about ten years ago, several methods for obtaining the exploring beam of the angular spread narrower than the angular range of selective reflexion have been devised, and by the use of double-crystal spectrometers applying these methods it becomes possible to measure the rocking curves which reproduce fairly closely the characteristics of the intrinsic ones. Broadly these methods are classified as follows:

(i) Limitation of a diffracted beam of the Laue case, which is spread in a crystal like a fan, by a slit placed behind the monochromator crystal (Borrmann & Kohra, 1959; Authier, 1960; Nakano, Kikuta & Kohra, 1964; Nakano, 1965).

(ii) Use of a diffracted beam of the Laue case, which is transmitted through a sufficiently thick crystal by the effect of anomalous transmission (Borrmann & Kohra, 1959).

(iii) A combination of (i) and (ii), in which a slit broader than that in (i) is used because, as pointed out by Nakano (1965), the diffraction effect due to the slit restricts the angular spread of the beam obtained in (i).

(iv) Use of a diffracted beam of the asymmetric Bragg-case (Renninger, 1961; Kohra, 1962).

Here it is worth while to mention the work of DuMond and his coworkers (DuMond, 1937; Bollman, Bailey & DuMond, 1938). He proposed the use of the beam diffracted successively by two crystals, the diffracting planes of which had the same spacing and were so slightly inclined that the reflective regions overlap only partly with each other. The angular width of the beam thus obtained is narrower than that of the intrinsic curve of the crystals concerned. Using this beam as the exploring beam in the arrangement corresponding to the double-crystal spectrometer of parallel setting*, they made some measurements of the rocking curves, but were able to observe neither the asymmetric profile nor the nearly flat region. This was, as they themselves presumed, probably because the tail of the

* Strictly speaking, the arrangement used by them is a triple-crystal spectrometer of the $(n, -n, n)$ setting.

Kazutake Kohra photographed in 2016 and the title page from an article that he published, along with Seishi Kikuta, in the first issue of *Acta Cryst. A*.

Kazutake Kohra, Professor Emeritus of the University of Tokyo, Japan, passed away on 31 January 2019 at the age of 97. After graduating from the University of Kyushu, he was appointed an Associate Professor at the University of Kyushu, and moved to the College of Arts and Sciences of the University of Tokyo in 1953. He spent two years (from September 1955 to December 1957) at the Fritz-Haber-Institut der Max-Planck-Gesellschaft in Berlin, Germany, when Max von Laue acted as its director. In 1963, he moved to the Department of Applied Physics in the Faculty of Engineering of the University of Tokyo and brought up many competent researchers who later on, up to now, have been working in the field of synchrotron radiation research.

Immediately after retiring from the University of Tokyo in 1979, he was appointed the first director of the Photon Factory, which was commissioned in 1982 at Tsukuba, Japan, as one of the first second-generation synchrotron radiation facilities in the world. The realization and success of the Photon Factory would have been impossible without the enormous leadership and great personality of Professor Kohra. He also acted as the first president of the Japanese Society of Synchrotron Radiation Research (JSSRR).

His primary research field was concerned with the dynamical theory of X-ray diffraction and its application to the observation of imperfections of crystals such as silicon and

quartz using X-ray topographic methods. The high-precision X-ray optics with multiple crystals that he developed have been highly regarded.



Group photo taken in Berlin in 1957. Back row from left to right: Kazutake Kohra, Max von Laue and Gerhard Borrmann. Front row from left to right: Mrs von Laue and Mrs Kohra.

Professor Kohra had very close contact with Dr von Laue during his two-year stay in Berlin (see photo above) and often talked about their valuable interactions to us students, which still remain deeply in myself.

We all appreciated the prominent research activities, enormous leadership and great personality of Professor Kohra, and mourn his loss.

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Search for papers by Kohra, K. in **Crystallography Journals Online**.

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OBITUARY

Michael G. Rossmann (1930–2019), pioneer in macromolecular and virus crystallography: scientist, mentor and friend

Eddy ArnoldHao WuJohn E. Johnson



Michael Rossmann holding a virus model at the Ninth Virus Assembly Meeting in Madeira, Portugal, in May 2018 (photograph courtesy of Roger Castells Graells, John Innes Institute, Norwich, UK).

Michael George Rossmann, who made monumental contributions to science, passed away peacefully in West Lafayette, Indiana, USA, on 14 May 2019 at the age of 88, following a courageous five-year battle with cancer. Michael was born in Frankfurt, Germany, on 30 July 1930. As a young boy, he emigrated to England with his mother just as World War II ignited. Michael was a highly innovative and energetic person, well known for his intensity, persistence and focus in pursuing his research goals. Michael was a towering figure in crystallography as a highly distinguished faculty member at Purdue University for 55 years. Michael made many seminal contributions to crystallography in a career that spanned the entirety of structural biology, beginning in the 1950s at Cambridge where the first protein structures were determined in the laboratories of Max Perutz (hemoglobin, 1960) and John Kendrew (myoglobin, 1958). Michael's work was central in establishing and defining the field of structural biology, which amazingly has described the structures of a vast array of complex biological molecules and assemblies in atomic detail. Knowledge of

three-dimensional biological structure has important biomedical significance including understanding the basis of health and disease at the molecular level, and facilitating the discovery of many drugs.

1. Education in crystallography with J. Monteath Robertson and William N. Lipscomb

Michael had enormous impact on developing methodology for the determination of macromolecular crystal structures. His grasp of mathematics was always a strength, as he continually developed methods that would become part of the standard repertoire of macromolecular crystallographic tools. Michael obtained undergraduate degrees in mathematics and physics at the University of London. For his graduate work, he studied crystal structures of organic compounds with J. Monteath Robertson at the University of Glasgow. Following his graduate studies he was a postdoctoral fellow with William N. Lipscomb at the University of Minnesota, USA, pursuing structures of relatively complicated organic crystals. In his work at Minnesota, Michael wrote computer programs (in machine language at the time) for crystal structure analysis, taking advantage of the new digital computers that would revolutionize the practice of crystallography. In a lecture by Dorothy Hodgkin at the Fourth IUCr Congress in Montreal in 1957, Michael learned about exciting work on the structure determination of hemoglobin by Max Perutz at Cambridge University. Michael wrote to Max and was given an offer to join the hemoglobin structure determination team.

2. Beginnings of protein structure determination at Cambridge

Michael worked closely with Max Perutz and was instrumental in elucidating the hemoglobin structure by writing the computer programs required to solve and analyze these first structures, and by calculating the Fourier maps that gave rise to the hemoglobin structure. Max had been pursuing the crystal structure of hemoglobin since the late 1930s and was a protégé of Sir Lawrence Bragg, one of the giants of crystallography who had helped to create the field of X-ray crystallography with his father, Sir William Bragg. When Michael arrived at Cambridge he began to analyze the X-ray diffraction data that Max and Ann Cullis had collected for the native hemoglobin crystals and multiple heavy-atom derivatives.

He invented methods and created computer algorithms for reliable phasing using heavy-atom isomorphous replacement and the practical determination of protein structures. While processing and analyzing the existing heavy-atom derivative datasets, he developed the difference Patterson map using squared difference coefficients $(|F_{\text{heavy}}| - |F_{\text{native}}|)^2$ to assist in locating the relative positions of heavy atoms in the isomorphous datasets (Rossmann, 1960). Michael also applied similar considerations to locating heavy atoms using anomalous dispersion (Rossmann, 1961) and with David Blow developed the single isomorphous replacement method (Blow & Rossmann, 1961) and mathematical representations of combining phase information from multiple sources (isomorphous replacement, anomalous dispersion *etc.*) (Rossmann & Blow, 1961). By 1959, Michael had computed a 5.5 Å resolution electron-density map for hemoglobin that permitted a trace of the overall fold of this predominantly helical protein and revealed its three-dimensional relationship with myoglobin (Perutz *et al.*, 1960).

3. Molecular replacement has become the most common method for solving macromolecular crystal structures

During his extraordinarily productive time at Cambridge, Michael also proposed and created the foundations for the molecular replacement method, which became the predominant approach for solving three-dimensional structures of proteins and other large biological assemblies such as complex enzymes and viruses. Michael had been fascinated with what he learned from conversations with other scientists at Cambridge, often during afternoon tea. For example, Crick and Watson had hypothesized that viruses would contain many identical protein subunits based on considerations of their limited genomic capacity (Crick & Watson, 1956). Michael thought that the recurrence of biological structure in different environments, whether in a structure with multiple subunits (oligomeric enzymes, viruses *etc.*) or in different crystals, would provide the ability to phase (*i.e.* correctly image) crystal structures. Michael thought that this information could be used to help solve the phase problem for these otherwise intractable systems. The monumental paper that Michael wrote together with David Blow (Rossmann & Blow, 1962) presented the rotation function as a method for demonstrating the presence of rotational non-crystallographic symmetry within a crystallographic asymmetric unit and determining relative orientations. Walter Hoppe (Hoppe, 1957) had also hinted at a convolution of a similar type to find the orientation of known molecular fragments and these ideas were implemented by Robert Huber (Huber, 1965). Michael developed the rotation function based on the realization that the Patterson function would contain multiple copies of vector sets corresponding to the different orientations of the repeating units within the crystal. Rotation of the Patterson function by the angle relating the repeated objects should give 'peaks' where these vector sets were coincident, and Michael demonstrated its utility by detecting the relative orientation of the α and β chains in horse hemoglobin crystals. Later he and others would develop methods for locating the position of objects in crystals, so-called translation functions. He went on to champion these ideas, while along the way determining the structures of many crucial enzymes and viruses.

Currently, the molecular replacement method is the most common approach used for solving new macromolecular structures, accounting for some 85%+ of all new PDB structure depositions and the majority of all 150 000+ known structures. Molecular replacement is most frequently used to determine the orientation and location of related structures in new crystals. The search model can be the same as the new structure, or a homolog with significant three-dimensional similarity. The initial phases can then be refined using the actual sequence corresponding to the new structure using a wide variety of phasing approaches including isomorphous replacement, density modification and ultimately atomic model refinement. Non-crystallographic symmetry averaging is especially powerful in refining phases and producing electron-density maps with great clarity, particularly with systems that have a high degree of symmetry such as viruses, and modern computer program systems have facilitated use of these approaches by making the process more convenient.

4. Conserved nucleotide-binding fold in glycolytic enzymes: the Rossmann fold and revolutionary concepts in molecular evolution

Michael moved to Purdue University in 1964 to develop his own research program and apply his innovative methods to solve important biological structures. By 1971 he had determined the structure of the largest protein to date, the enzyme lactate dehydrogenase (Adams *et al.*, 1970). Within a few years he solved another related glycolytic enzyme, lobster glyceraldehyde-3-phosphate dehydrogenase, and showed unexpectedly that a portion of the structures that bound nucleotide cofactors had highly similar structures. Based on these observations he suggested that the architecture of proteins evolved in the same way as the anatomy of animals (Buehner *et al.*, 1973; Rossmann *et al.*, 1974). This conserved part of protein anatomy is called the 'Rossmann fold' to recognize Michael's ingenious new idea. He had initially thought along these lines at Cambridge: when solving the structure of hemoglobin, a protein that carries oxygen in red blood cells, Michael saw that the two protein chains of hemoglobin had strong three-dimensional resemblance to each other despite lacking obvious sequence similarity, and also to myoglobin, which carries oxygen in muscle tissues. Although these concepts are very well accepted now, Michael's ideas often were greeted with resistance because they were revolutionary when suggested.

5. Passion for viruses: technology and a plant virus structure

A driving force behind Michael's interest in pursuing more and more complicated biological structures and in technology development was his passion to study virus structure. Michael subsequently pioneered the structure solution of entire viruses in atomic detail, requiring considerable advances in technology to handle the larger unit cells and massive amounts of crystallographic data. Following the publication of the tomato bushy stunt virus structure (Harrison *et al.*, 1978) from Stephen Harrison's group in 1978, Michael reported the structure of Southern bean mosaic virus (Abad-Zapatero *et al*., 1980), and the surprising revelation that the coat protein structures of these two plant viruses shared a common protein fold, an eight-stranded β-barrel also known as a 'jelly roll' fold. This work required the development of oscillation photography for data collection, and processing and post-refinement of the intensity data measured on X-ray film (Rossmann *et al.*, 1979; Winkler *et al.*, 1979). Writing programs and developing efficient algorithms for location of heavy atoms in the presence of non-crystallographic symmetry and averaging of the electron density were also massive undertakings, especially given the more limited computing resources of that era.

6. The common cold virus structure: more innovations and amazing biology

Michael shifted attention to animal viruses in the early 1980s. His work gained wide attention when he reported the structure of a common cold virus in 1985, human rhinovirus 14, the first animal virus described in atomic detail (Rossmann *et al*., 1985). The rhinovirus structure was a landmark in terms of its biological significance, illuminating principles of viral assembly, and interactions with neutralizing antibodies, cellular receptors and antiviral drugs. Michael’s career-long theme of making fundamental discoveries in molecular evolution struck once again – the coat protein structures of

human rhinovirus 14 showed great similarity to the plant virus structures, in spite of having essentially no detectable sequence conservation!

The structure determination of rhinovirus itself was extraordinary, using a pioneering combination of high-intensity synchrotron radiation, high-speed supercomputing and the most convincing demonstration up to that time of phase extension using non-crystallographic symmetry averaging and reconstruction (Arnold *et al*., 1987). Heavy-atom phases were only available to 5 Å resolution from a single $Au(CN)_2$ derivative, and phase extension via 20-fold non-crystallographic symmetry averaging and reconstruction in gradual steps to 3.5 Å resolution led to a complete trace of the four chains of VP1, VP2, VP3 and VP4 in the protomeric unit. Within three weeks a complete model of the >800 amino acids in the icosahedral asymmetric unit had been built using a newly acquired Evans & Sutherland computer graphics system. The phase extension was carried out to 3.0 Å resolution, and the refined phases were subsequently used as observations in atomic model refinement because of their accuracy (Arnold & Rossmann, 1988). Some of the current cryo-electron microscopy (cryo-EM) model refinements using the observed phases have adopted a similar methodological approach, where phases obtained experimentally from the EM determination are used as observations in reciprocal space-based refinement protocols. A great deal of programming was required to adapt the Rossmann laboratory software from earlier CDC6000 series computers (CDC6500 and CDC6600) to the Cyber 205 supercomputer, and many memorable adventures occurred during that process, including finding and fixing ‘bugs’ in the programs that sometimes may have existed since their initial implementations!

7. Virus structures for all seasons and initial work using cryo-EM

Following the common cold virus structure work, Michael solved the crystallographic structures of many other RNA viruses from plants and animals including polio-, coxsackie-, and cardioviruses. He also determined the crystal structures of DNA viruses including human, canine, feline and porcine parvoviruses. In addition, Michael solved the detailed structures of both small and large bacteriophages. To further probe biological function, Michael pursued the structures of complexes of viruses with their cellular receptors, neutralizing antibodies and small-molecule drugs. To study some of the complexes with cellular receptors and antibodies, Michael began to use cryo-EM. Tim Baker had set up an experimental facility at Purdue University for the study of virus structure by cryo-EM and, with Jack Johnson, studied interactions between plant viruses and cognate antibodies as a proof-of-concept for the study of such complexes (Wang *et al*., 1992). Michael and Baker used this approach to show that the ICAM-1 receptor for HRV14 bound in the canyon as predicted (Olson *et al*., 1993). In addition, Tom Smith and Baker studied a series of monoclonal Fab fragments attached to their cognate antigenic sites on HRV14.

8. Cryo-EM: large and enveloped viruses including the flavivirus structures

As many viruses cannot be crystallized easily, Michael also recognized, fairly early on, the importance of cryo-EM for structural virology. When cryo-EM investigations can be augmented by crystallographic determination of the component proteins, they produce ‘pseudo atomic resolution’ structures of the whole virus, a method dubbed hybrid technology that Michael helped to develop. Today, cryo-EM is capable of producing high-

resolution structures providing atomic detail with suitable samples, but during the 1990s the cryo-EM technology was limited to producing structures of viruses and other assemblies at resolutions in the 10–20 Å range, and the hybrid method was the approach that could provide interpretation of interactions as the molecular level of detail. With Tim Baker, Michael was able to use the hybrid method to determine the structure of the lipid enveloped alphaviruses Ross River virus (Cheng *et al*., 2002) and Sindbis virus (Zhang *et al*., 2002). Together with virologist Richard Kuhn who had joined the Purdue structural biology group, Michael determined the structures of flaviviruses, *e.g.* dengue virus (Kuhn *et al*., 2002) and West Nile virus (Mukhopadhyay *et al.*, 2003), and mapped their interactions with antibodies and conformational changes when subjected to acidic conditions. In the astonishing Zika virus work, he and collaborator Richard Kuhn obtained a sample of the virus in February 2016 and published the complete atomic structure in *Science* in April (Sirohi *et al*., 2016). Michael's laboratory was equipped by this time with state-of-the-art cryo-EM technology (Titan Krios and Gatan K2 Summit detector) underlying the 'resolution revolution' in EM that permits high-resolution structure determination of complex macromolecular structures from averaging of many thousands of randomly oriented single particles or viruses. As was characteristic for him throughout his research career when working on new topics and technological areas, Michael wrote computer programs to perform EM analyses including obtaining optimal fits of atomic models into cryo-EM electron-density maps. Over time, Michael also became emphatic that crystallography was 'old fashioned' and that cryo-EM was the wave of the future. But when good crystals can be obtained, there can be many advantages to solving crystal structures, especially given the extraordinary technological innovations that have occurred in this field, among which are synchrotrons, 100% quantum-efficient detectors, very powerful and flexible software packages and tremendously faster computing hardware along with massive data storage systems with rapid access.

9. Awards, honors, recognitions, and honorary degrees

Michael's achievements, which have been recognized by many awards, are among the most impactful contributions to the chemical and life sciences: inventing crystallographic methodology used to solve most macromolecular structures; solving virus structures and developing the methods for doing so; and suggesting that proteins could evolve, with folded domains being the fundamental evolutionary unit. Michael was a Member of the US National Academy of Sciences (1984) and the American Academy of Arts and Sciences (1978), and was a Foreign Member of the Royal Society (1996). Among his most notable awards were the Ewald Prize, Gregori Aminoff Prize, Fankuchen Award, Louisa Gross Horwitz Prize, Gairdner Foundation Award, Paul Ehrlich and Ludwig Darmstaedter Prize, Sackler Prize in Biophysics, Stein and Moore Award from the Protein Society, and three consecutive NIH MERIT Awards. He held six honorary degrees from international universities and was a Member of the National Science Board (2000–2006), having been nominated by President Bill Clinton.

10. Crystallographic awards and contributions to education in crystallography

Michael was especially proud that the Ewald Prize (1996), the highest award given by the IUCr only once every three years, recognized his inventions in crystallographic

methodology, including the molecular replacement method. The Fankuchen Award from the American Crystallographic Association (1986) was also especially fitting because Isador Fankuchen published the first diffraction patterns from virus crystals. Together Michael and Eddy Arnold edited Volume F of the *International Tables for Crystallography*, which was the first volume of the series that focused on macromolecular crystallography (Rossmann & Arnold, 2001). The first edition was published in 2001, with a second in 2012 including contributions from Daniel Himmel (Arnold *et al*., 2012), and a third is in preparation with the participation of Liang Tong. The third edition will be dedicated to the memory of Michael.

Michael trained a legion of scientists, including postdoctoral and graduate students who themselves have established many vibrant and productive research programs worldwide. Michael developed many close life-long friendships with his students and co-workers. Michael also played a key role in the education of young scientists in crystallography and structural biology. For example, he organized the first meeting of the International School for Crystallography in Erice, Italy, on the topic of macromolecular crystallography in 1976, when Dorothy Hodgkin was the Director. In 2006, Michael again organized the school on the topic of biological macromolecules and their assemblies, with Tom Blundell as Director of the School. The 2006 program included a strong representation of the field of cryo-EM, reflecting Michael's interest in using that approach to image biological structures of ever-increasing complexity. The Erice school often has as many as 100 or more students at the graduate and postdoctoral level in attendance for a ten-day program that features a mix of talks on fundamental methodology and new results.

11. Michael's family life

Michael and his dear wife of 55 years, Audrey, had three children. In addition to son Martin, and daughters Alice and Heather, he is also survived by four grandchildren. Following Audrey's death, Michael met Karen Bogan. They were married a year ago and enjoyed great happiness together. At a Memorial Service in West Lafayette, following his death, many memories of him as a warm and influential family member, friend and mentor were shared, including his child-like curiosity about almost everything and diverse interests in exploring the natural world, both physically and intellectually.

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This obituary was originally published in *Acta Cryst.* (2019). D**75**, 523–527.

Original article: https://www.iucr.org/news/newsletter/etc/articles?issue=142706&result_138339_result_page=36

OBITUARY

An-Pang Tsai (1958-2019)

Marc de Boissieu

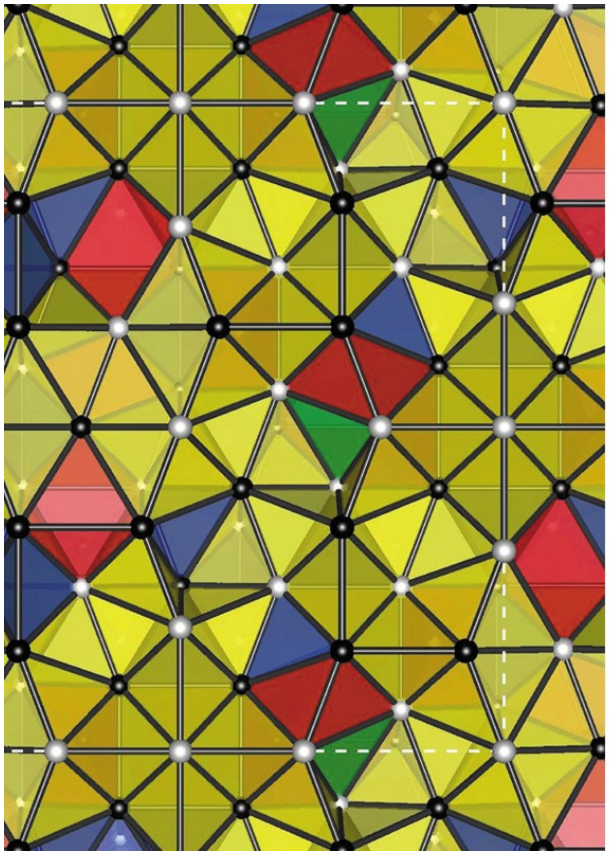


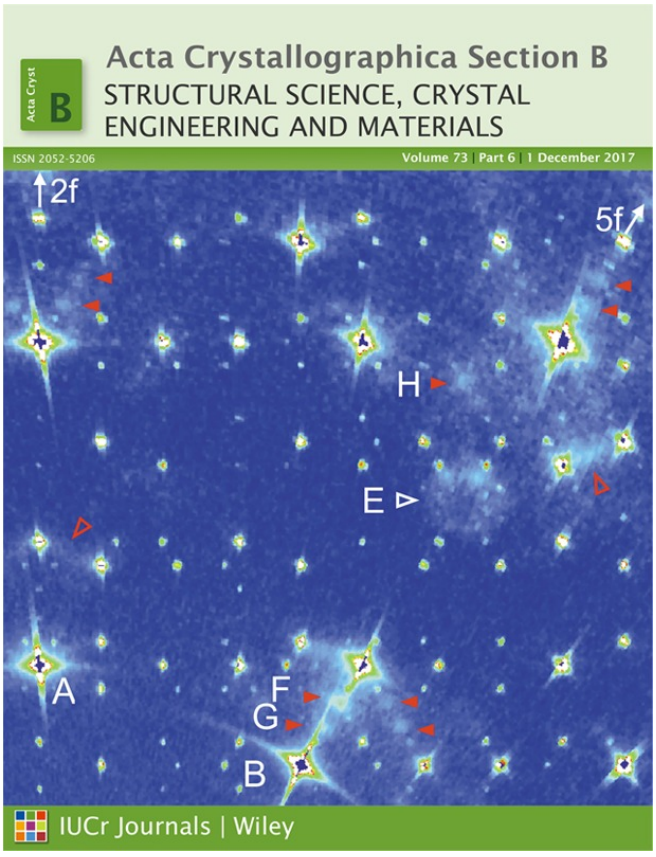
It is with great sadness that we report the passing away of An-Pang Tsai on 25 May 2019 at the age of 60.

He was a professor at Tohoku University, Sendai, Japan, and a leader in the field of quasicrystal and complex intermetallic research. His discovery of most of the known stable quasicrystals has been invaluable in understanding the structure and physical properties of these aperiodic crystals. Professor Tsai received many awards including the Medal of Honor with Purple Ribbon bestowed by the Japanese government.

He will be sorely missed by his many friends and colleagues in the crystallographic community. Our thoughts go to his wife, children and family.

A full obituary has been published in *Acta Cryst. B*.





Images from IUCr Journal articles co-authored by Professor Tsai. Left: Cluster-packing geometry for Al-based F-type icosahedral alloys, right: Atomic structures of ternary Yb–Cd–Mg icosahedral quasicrystals and a 1/1 approximant.

Original article: https://www.iucr.org/news/newsletter/etc/articles?issue=142706&result_138339_result_page=37

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

Original article: https://www.iucr.org/news/newsletter/etc/articles?issue=142706&result_138339_result_page=38

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

Original article: https://www.iucr.org/news/newsletter/etc/articles?issue=142706&result_138339_result_page=39

Small ads



Georg-August-Universität Göttingen
Stiftung Öffentlichen Rechts

The Faculty of Chemistry wishes to appoint a

Junior professor (W1) for Inorganic Structure Analysis and Molecular Interaction (Bes.Gr. W 1 NBesO)

to commence on the January, 1st, 2020. The appointment is for three years, with a possible extension for further three years.

The professor is expected to perform research and teaching in inorganic chemistry. Applicants should be recognized for excellent achievements in a modern area of Xray diffraction analysis. The position will be located within the Institute of Inorganic Chemistry and suitably complement the faculty interdisciplinary focal research area of Analytical Methods on Molecular Interaction. Experience in one of the contemporary areas as photo crystallography, high- or time-resolved crystallography is requested. Participation in existing (GRK 2455) and planned research initiatives of the Faculty of Chemistry is requested. Participation in academic administration is mandatory. The University of Göttingen emphasizes research-oriented teaching.

The requirements of appointment are specified by §30 of the "Niedersächsisches Hochschulgesetz" (NHG) (Nds. GVBI. 2007 S. 69). In case you have been employed as a scientific employee, or scientific teaching assistant, before or after receiving the Ph.D. degree, the total time of employment and Ph.D. studies should not exceed 6 years. Further details can be found at § 26 NHG and will be clarified upon request.

Applications from scientists working abroad are particularly welcome. Applications of disabled persons will be given preferential treatment over other candidates with equal qualifications. The University aims to increase the percentage of women in areas in which they are under-represented and thus encourages suitably qualified women to apply.

Online applications with CV, publications list and details of teaching and research experience should be received by June, 30th, 2019. Applications by regular mail are accepted.

Online link for applications and further information: http://www.unigoettingen.de/en/607063.html

Please note: With submission of your application, you accept the processing of your applicant data in terms of data-protection law. Further information on the legal basis and data usage is provided in the https://www.unigoettingen.de/hinweisdsgvo

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