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LETTER FROM THE PRESIDENT

IUCr Commissions - our guiding light

Sven Lidin



The IUCr Commission on Crystallography in Art and Cultural Heritage (CrysAC) co-organized the IUCr2017 exhibition "Beauty Hidden in Rocks" with geologist and photomicrographer Bernardo Cesare. Shown are CrysAC members Gilberto Artioli (left) and Alicja Rafalska-Lasocha along with Michele Zema, IUCr Executive Outreach Officer.

The IUCr is a chimera, a hybrid beast with diverse aspects. Very much like the lichens that are symbiotic organisms consisting of fungi cohabitating with a photosynthetic partner, it is a scientific union assuming the role of a publishing house and it is a publishing house assuming the role of a scientific union.

This state of affairs is highly beneficial to both aspects of the Union. As in the lichens, the different nature of the components makes them complementary and it is clear that the backing of the Union contributes to the high standing of the journals in our community and that the service the journals provide to the Union as a means of disseminating new results in appropriate channels with expert review systems and editing contributes to the relevance of the Union to its adherents.

The scientific union and the journals have grown together to become inseparable and the channels between these two aspects have developed over time. Among the most important are the [Commissions](#). The Commissions are fora for discussions of where the different branches of crystallography are headed and through the Commissions, the Union gets intelligence on where to turn in an ever-more rapidly changing scientific landscape. The Commissions form an integral part of the Programme Committee for the IUCr Congress and they organize specialized meetings and workshops within their respective areas of expertise. They are simply excellent antennae tuned to the future of the Union.

Our commissions are, however, somewhat vulnerable. They consist of a limited number of individuals who should represent the breadth of the subject and, taking gender balance into account, should also reflect the geographical spread of the Union. The Executive Committee is considering ways to strengthen the structure of the Commissions to make them more robust but in the end, the only way to guarantee strong commissions is to have good proposals for new membership as continuity and renewal of our Commissions is vital to the health of the Union.

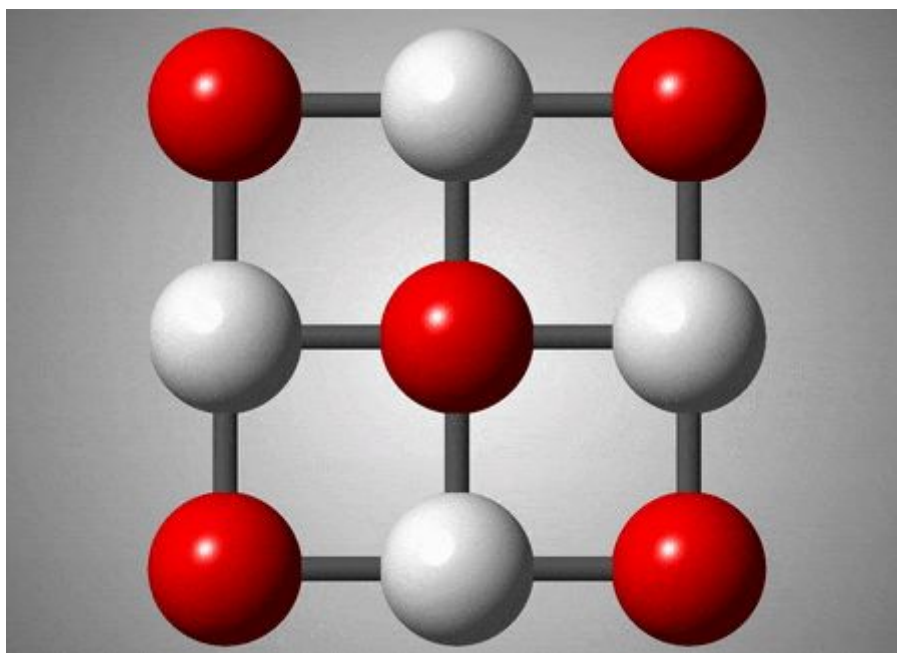
Nomination for Commission membership may come from the Commissions themselves but in order to propose new membership, the National Committees have a key role. Through nominations made by the National Committees, the IUCr has a mechanism to identify suitable Commission members with the ability and willingness to do the work essential for the well-being of the Union.

The next General Assembly is rapidly approaching and I urge all of you to think carefully about which new members of our Commissions would fit that bill and to contact your [National Committees](#) with your suggestions.

EDITORIAL

Editorial

Mike Glazer



The summer here in the northern hemisphere is now almost over and I guess everyone will be returning from holidays (or conferences?) to get back to work. Here in the UK, the academic term will be starting in October and the yearly routine will begin again. Although I retired officially nine years ago, I still look forward to meeting and teaching the next intake of students. I guess it is the opportunity to talk to the next generation that keeps me young and beautiful.

I recently attended the European Crystallography Meeting in Vienna, Austria, and was struck by the huge number of participants from all over the world, not just from Europe. The setting for the meeting of course was stunning: how could it not be in a wonderful city like Vienna? It was a particular pleasure to have the meeting at the University of Vienna, where one of my scientific heroes, Ludwig Boltzmann, had worked. For crystallographers, it was also the place where Max Perutz was educated. The list of great scientists is almost endless.

At the ECM, Robert Krickl once again exhibited his huge model of sodium chloride, this time bigger than ever. [First shown in 2015](#), the model subsequently made it into the *Guinness World Records*. Robert has now added extra balls to gain a new world record. He talks about this [here](#).

In this issue of the *IUCr Newsletter* we have yet another [contribution](#) from Massimo Nespolo, which, as usual, is well worth reading. This time he discusses the confusion in the literature to do with the terms super- and sublattice, super- and subcell and super- and substructure. Did you know that the lattice corresponding to a superstructure is actually a sublattice? The most common mistake that I see in the literature is the use of the term superlattice when what is meant is actually superstructure. This is yet another example of the muddle between lattice and structure, as already explained in the previous [Newsletter](#). In crystallography the IUCr spends a huge amount of effort to make sure that crystallographic terminology is defined as rigorously as possible but unfortunately, there is a lot of sloppy usage out there.

I have this time also added an [article](#) about a Hollywood film in which our subject "crystallography" gets a mention, which I hope will intrigue you. The film was made in 1951 in England and one has to ask why was crystallography mentioned at all? I suggest a reason in the article.

We also have a [contribution](#) from John Helliwell addressing the question of the importance of protein crystallography in biology. Reporting of protein crystal structures, and their associated database entries, could usefully indicate how close they are to the biological situation, e.g. room temperature is better than cryo etc., as discussed in detail in the article.

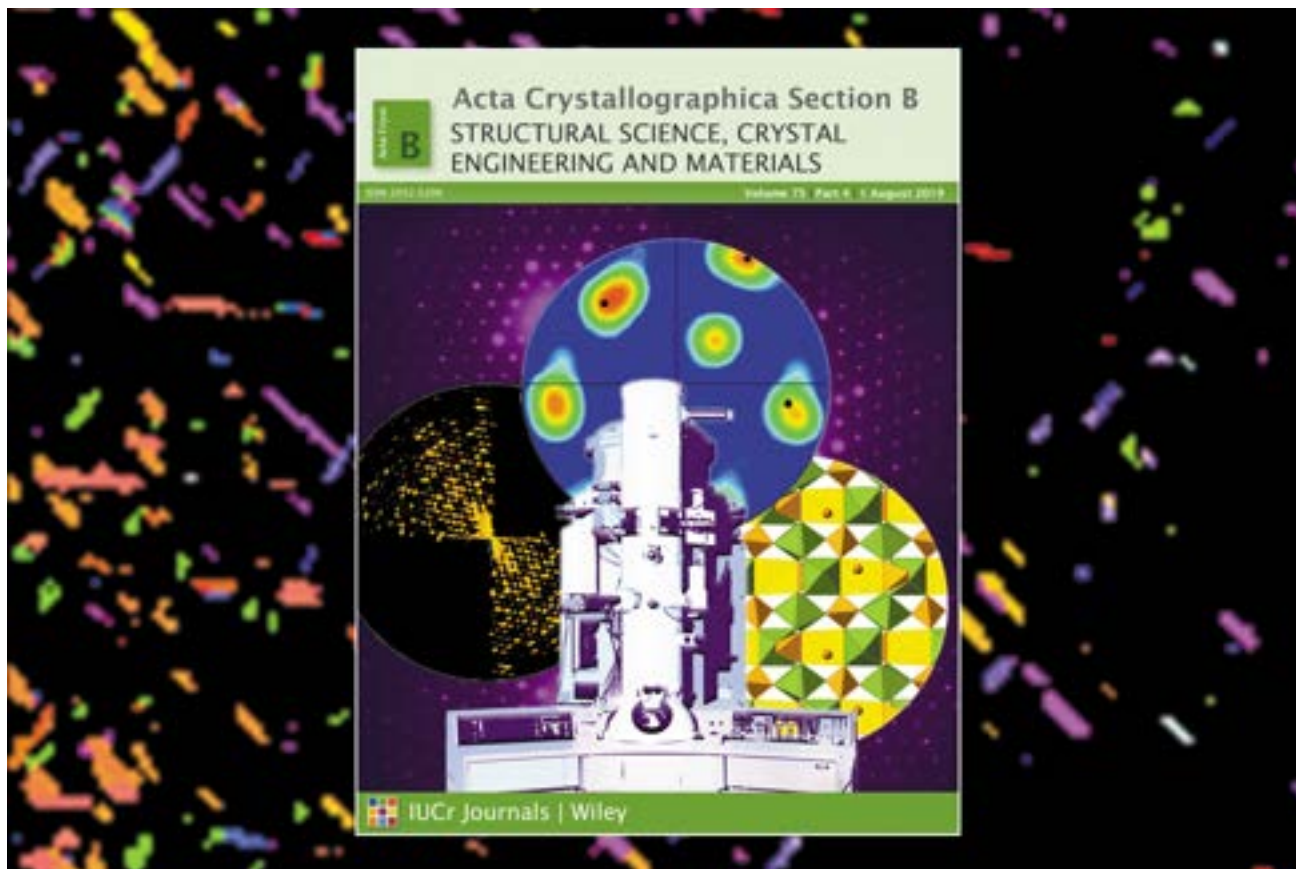
I hope you will enjoy the film created by Richard Welberry of [quasiperiodic arrays](#). Richard explains the background theory and how one can create these images for yourself if you are a Mac user.

Finally, we [report](#) the sad death of Carl Schwalbe, American by birth but living for many years in the UK. I knew Carl quite well, both here in the UK at our British Crystallographic Association meetings, but also when our paths crossed at Harvard in 1968 to 1969, where he was working on his PhD under Bill Lipscomb.

IUCR JOURNALS NEWS

Acta Cryst. B: Electron crystallography special issue

Joke Hadermann Lukáš Palatinus



Structure analysis of micro- and nanocrystalline materials has witnessed immense progress in the last decade thanks to the development of electron diffraction techniques. The automation of data collection, development of new data collection modes and improvements in the data treatment have allowed unprecedented progress in most aspects of crystallography dealing with very small crystals. Probably the most notable change of paradigm is observable in the structure determination of unknown phases by electron diffraction. Three-dimensional diffraction techniques now allow almost routine solution and of structures from single crystals as small as a few tens of nanometres, providing access to hitherto unsolvable crystal structures or to previously unattainable level of structural detail. Scanning diffraction techniques allow phase and orientation mapping with nanometre resolution and even three-dimensional reconstruction of phase and orientation distributions.

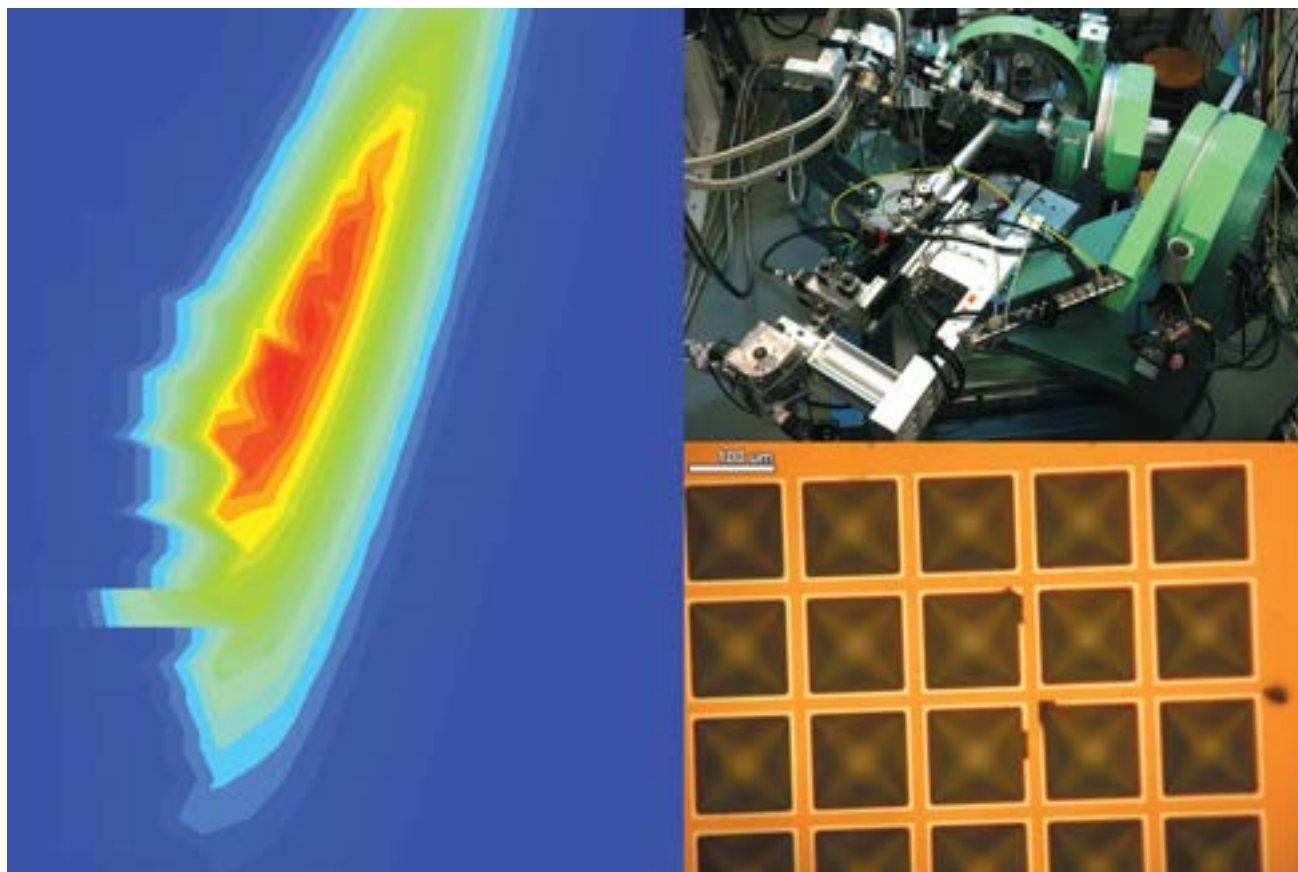
This [special issue of Acta Cryst. B](#) features a collection of original contributions covering a broad range of aspects of electron crystallography. An interested reader will find papers describing the foundations and methodological basis of structure solution by electron diffraction, theoretical and methodological advances in data processing, discussion of applications of electron diffraction outside the realm of perfectly periodic crystals as well as specific case studies showing the application of the methods to hot topics in current crystallography.

The collection of contributions in this special issue showcases the diversity of applications of current electron diffraction techniques, demonstrates the state of the development of the technique and also features work that further advances the electron diffraction methods. We believe that this special issue can serve as a starting point for anybody interested in electron crystallography and we are convinced that the contributions in this issue will become reference points for future research in this exciting field.

EDITORIAL

Large-science facilities must continue to add value to the scientific community

Dimitri N. Argyriou



The main arguments that drive investment in large-science facilities are the new scientific insights that will be gained by significantly enhanced technical performance. The case for free electron lasers (FELs), for example, is made on unprecedented generation of photons with a unique time structure, which allow researchers to see inside single molecules. Similarly, snappy '*science cases*' are made for both the Large Hadron Collider at CERN and the European Spallation Source in Lund, Sweden. However, with highly visible costs to run large-science facilities, university researchers, and rightly so, do challenge these commitments, with the often-heard argument of '*give me the money instead and I will spend it on real science!*'. While university funding should be a priority, the real question being asked is '*Do large-science facilities provide value for making progress in science?*'. This question is now becoming even more pressing as new advances provide highly impactful tools for scientific discovery, at a price that most well-funded universities can afford.

Advanced technical performance provided by large-science facilities alone is not sufficient to either justify the investment or sustain substantial long-term operational costs. The true value of these facilities is harnessed over many decades by an engaged scientific community, especially when the facility becomes an integral component of that community. That impact is clear when viewing the stream of key scientific results they have provided over the decades and the support they have contributed for breakthrough Nobel-Prize-winning work (such as work on soft-mode transitions, spin excitation in superconductors, glass transitions, magnetic monopoles, protein structures and fast dynamics). Their

impact also goes beyond the scientific results alone by often developing technologies that have wide societal impact (html, capacitive displays, modern cryostats and many others).

Value is an abstract concept and hard to generalize as it varies between researchers and scientific communities. For some, it may be as simple as the opportunity for a nearby ski-trip after attending an experiment at a facility. For most, there are the added benefits of unique measurements that are not charged to your research grant. A user of a large-science facility gets a lot of added value in terms of free support; this can include software and experimental support, consumables such as liquid He, sometimes paid travel, opportunities to network and attend important seminars, cost sharing on students *etc.* Indeed, some universities acknowledge this added value by treating accepted beamtime proposals as grants into their departments. And, yes, these hard to come by measurements can be a career launch pad for many young scientists.

While this large-science business model of providing unique scientific capability combined with high-quality scientific and technical support has worked for many decades, it is now challenged on two fronts. The first front comes from continual technical innovation and development, which can deliver high-profile impactful science at an affordable price to most well-funded universities. Cryo-electron microscopy is one example, but others exist such as laser-ARPES (a technique usually performed at synchrotrons), magnetic imaging using Lorentz lenses in electron microscopes (a technique that can compete with experiments performed at neutron sources), quantum sensing and computing. New laboratory X-ray equipment can now routinely provide third-generation synchrotron performance. Investments in these new technologies runs at a broad but affordable price scale of 500k to 15M USD. The advantages are clear, potentially highly impactful scientific results, easy access for local researchers, unique capabilities and ability to control future scientific and technical directions. The argument that this competitive advantage is lost if everyone has access to such capabilities misses the point that the advantage often lies in timing of research, the sample examined and the skill of the researchers. The actual case to justify these investments by universities is that, if they do not invest in these powerful and affordable tools, they will not be able to attract top talent or remain scientifically competitive.

The second challenge to the facility business models comes from their own success, in the form of mission or scope creep. At facility reviews, the most hotly discussed areas after the number of beam days provided to users and the number of high-impact publications, are all value-added science support items such as data analysis, support for sample environment *etc.* It is natural, of course, given the position of many large-scale facilities at the nexus of scientific and technological advances, to try to drive innovation in many key areas that enable new science. Facilities also benefit from resources, engineering expertise and project management skills to drive that technological innovation. However, in order to remain competitive and add value, the potential for upward scope creep is clearly evident. This can include sample preparation and characterization laboratories, deuteration facilities, high-pressure facilities, high-performance computing infrastructure – the list grows continually. The diversity and size of scope that adds value, and is demanded by the community, is significant and facilities are stretched to their very limits to satisfy these demands.

With the technological development of affordable and impactful laboratory-based tools and their ever-growing scientific scope, large-science facilities need to review their strategies in order to continue to add value for their scientific communities. To ensure success, facilities will need to be fully cognizant of the scientific and technological developments that are taking place outside their own domain. Competitive analysis with techniques available at an affordable price to universities will be needed in order to drive priorities and new investments. New strategies to remain competitive will likely challenge some established fields that have had a long-term presence in large-scale facilities, but perhaps are best served now by other means. Creating that headroom to allow for new innovations and investment for these new strategies, is essential in order to develop new opportunities that will continue to add value to the scientific community for the next decades. What is also essential is enhancing and possibly

rethinking engagement with scientific communities, perhaps even giving these communities a greater role in the value-chain of large-science facilities.

Acknowledgements

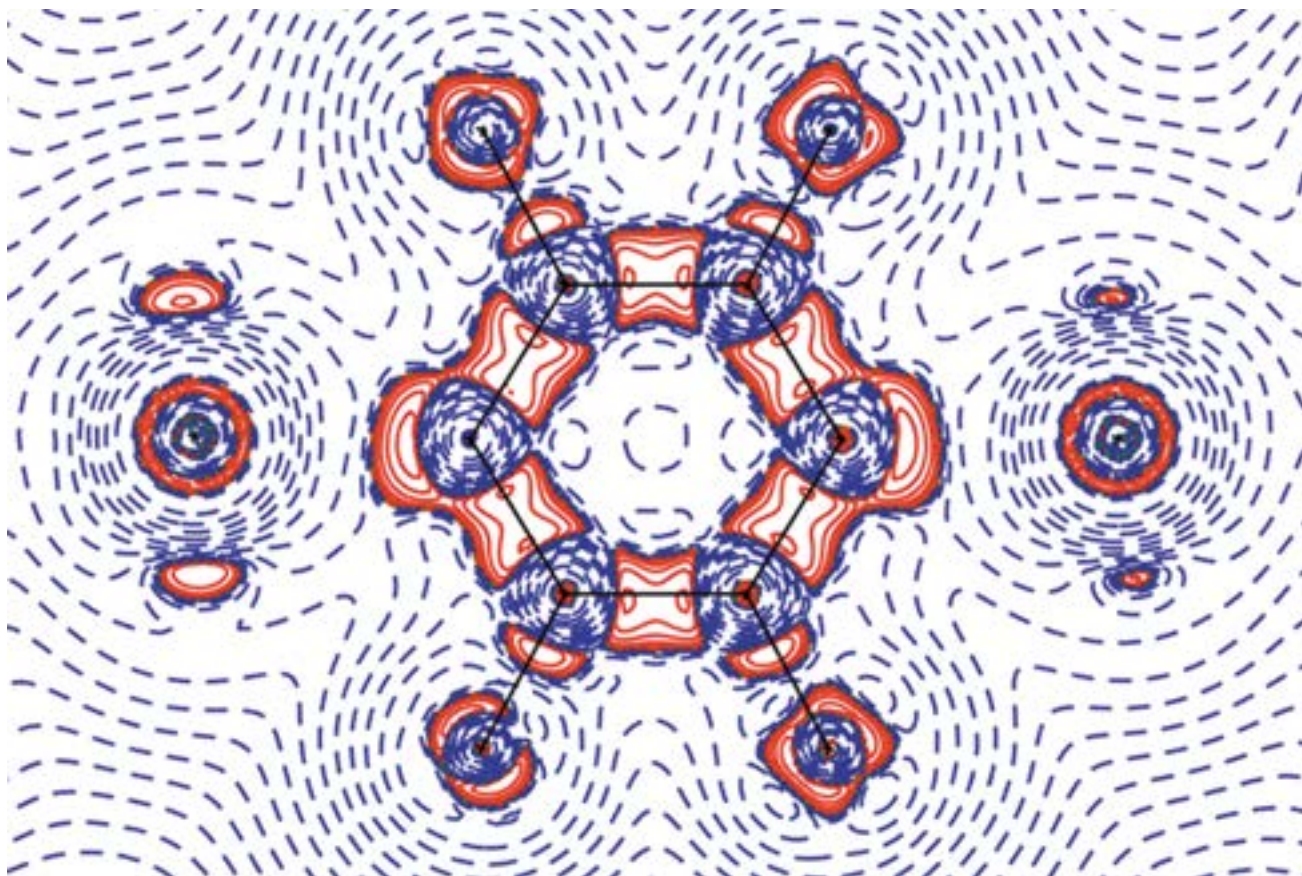
The author thanks Masa Arai and Heloisa Nunes Bordallo for critical comments.

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RESEARCH NEWS

A smorgasbord of halogen bonds?

Gautam R. Desiraju



In the beginning, hydrogen bonds were supposedly simple (Hüttermann, 2019), but life got more interesting as time went along. Who would have thought, for example, 100 years ago, when the hydrogen bond was first invoked, that we would be discussing $C-H\cdots\pi$ interactions (Nishio *et al.*, 1998), in acetylene and benzene, and that we would be calling one of them a hydrogen bond and the other a van der Waals interaction? And what does one make of dihydrogen bonds? In the past, no one even knew that they existed (Bakhmutov, 2008).

In fact, this latter example is one of the rare cases where a halogen bond, of say the type $Cl\cdots Cl$, was identified and recognized long before its hydrogen-bond analog, *i.e.* $H\cdots H$, was even thought of. It just goes to show, and in part it is because of such thought exchanges, that there has been a tendency to liken halogen bonds to hydrogen bonds. This simplification certainly helped in the formal definition of the term 'halogen bond' where it was held that an electrophilic halogen atom is a *sine qua non* for a true halogen bond (Desiraju *et al.*, 2013). But, on the other hand, this kind of comparison has also led to an inevitable tendency to think of the halogen bond as some sort of hydrogen bond with a halogen atom instead of the hydrogen. This is not quite accurate, and this is why we titled a review paper we wrote in 2013, 'Halogen bonds in crystal engineering: like hydrogen bonds yet different' (Mukherjee *et al.*, 2014).

We tend to think of many intermolecular interactions in terms of electrostatics, but we need also to think of atom size. Halogen atoms, especially iodine, the one under discussion in an article by Wang *et al.* (2019) in the September issue of *Acta Crystallographica Section C*, can become quite large, and steric factors apart, this means that the degree of symmetry in the electronic distribution within an atom can

be quite varied. The authors of the paper under consideration here have described, in fair detail, the charge-density and spectroscopic properties of a pair of I $\cdots$ N-containing cocrystals of 1,2,4,5-tetrafluoro-3,6-diiodobenzene with two different N-bases. The I $\cdots$ N distances are practically the same but the charge-density properties are different. Generally, the shorter a hydrogen bond gets, the stronger it gets. In this connection, one hears occasionally of breakdowns in this length-strength analogy in crystals (Braga *et al.*, 1998), but in these cases there seem to be other extenuating circumstances. In the pair of cocrystals described here, however, there is a clear breakdown of this analogy for the I $\cdots$ N halogen bonds, at least if one goes by the charge-density results. The interactions are of nearly equal length, but as far as bond critical point (bcp) characteristics go, they would appear to be of differing strengths. It is shown that the use of another technique, in this case Raman spectroscopy, provides a clearer picture of this complex interaction. Perhaps the bcp alone is not a complete enough descriptor of halogen-bond strength.

The differences between the two title compounds have mainly to do with the polarization of the I-atom electron density in the two cases. Iodine is very different from the other halogens. The authors make an interesting comment, almost in passing, that bromine might not be a good *via media* between chlorine and iodine when one discusses halogen bonds, although this statement is made in the context of halogen-atom diffraction. In a general sense though, I have found this not to be so – bromine in fact did provide a good enough approximation, but possibly this issue will be better resolved in the future.

The key feature here is that the two halogen-bond acceptor sites, an aromatic nitrogen in 4-(dimethylamino)pyridine and an alicyclic nitrogen in DABCO, differ greatly. They differ appreciably in their basicity and hence will have distinct effects on the highly polarizable iodine even at nearly equal interatomic distances. Furthermore, their differing chemical situation will also render them to be of differing polarizability. The DABCO N atom possesses greater polarizing power than the pyridine N atom; iodine is highly polarizable additionally and therefore there is a skewed electronic distribution on the I atom, leading to a so-called σ -hole in the DABCO case. The Laplacian values in the two cases also point towards a higher covalent character in the pyridine case than in the DABCO case. This is reflected in the V/G ratios mentioned in the article. Theoretical calculations generally fail to describe this effect properly due to a poor description of the electronic distribution for a heavy atom like iodine, but this is recognized by the authors. The high polarizability of iodine when compared to the other halogens is the critical attenuating factor which is responsible for the effects seen in the electron-density distributions in the two cases. Possibly such an effect might not be seen so easily for the corresponding Br $\cdots$ N interactions.

This article is worth highlighting because it opens up new opportunities in the charge-density and crystal engineering fields and in the overlap region between these fields. There is an urgent need to improve our charge-density modelling capabilities for heavy atoms. The lack of such a capability will hinder our progress in understanding halogen bonds. A great deal more needs to be done in terms of just reporting a greater variety of halogen bonds: our data bank of halogen bonds is still too small. The present paper is a one-off result and of course iodine is a special case. I would really like to see a lot more done with chlorine, which I personally believe to be the most challenging halogen with respect to the study of halogen bonds. The authors do not say much on the nature of the (3,–1) bcp *versus* Cl $\cdots$ Cl distance in terms of the type-I and type-II classification (Desiraju & Parthasarathy, 1989). Do the shorter contacts correspond mostly to type-II?

In the end, even hydrogen bonds are complex interactions: one needs to deal with electrostatics, covalency, polarization and dispersion before one begins to come to grips with the beast itself (Desiraju, 2002). The chances are that one is dealing with the same quartet of effects in a halogen bond, and it is likely that one needs many more examples before one is able to come up with a more complete description of the halogen bond. But in the end, we took about 100 years to get where we got with the hydrogen bond – and so we probably need to spend a little more time studying its halogen atom equivalent.

Acknowledgements

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References

Bakhmutov, V. I. (2008). In *Dihydrogen Bonds. Principles, Experiments and Application*. New York: Wiley-Interscience.

Braga, D., Grepioni, F., Tagliavini, E., Novoa, J. J. & Mota, F. (1998). *New. J. Chem.* **22**, 755–757.

Desiraju, G. R. (2002). *Acc. Chem. Res.* **35**, 565–573.

Desiraju, G. R., Ho, P. S., Kloo, L., Legon, A. C., Marquardt, R., Metrangolo, P., Politzer, P., Resnati, G. & Rissanen, K. (2013). *Pure Appl. Chem.* **85**, 1711–1713.

Desiraju, G. R. & Parthasarathy, R. (1989). *J. Am. Chem. Soc.* **111**, 8725–8726.

Hüttermann, A. (2019). In *The Hydrogen Bond. A Bond for Life*. Berlin: De Gruyter.

Mukherjee, A., Tothadi, S. & Desiraju, G. R. (2014). *Acc. Chem. Res.* **47**, 2514–2524.

Nishio, M., Hirota, M. & Umezawa, Y. (1998). In *The CH/π Interaction. Evidence, Nature, and Consequences*. New York: Wiley-VCH.

Wang, R., George, J., Potts, S. K., Kremer, M., Dronskowski, R. & Englert, U. (2019). *Acta Cryst.* **75**, 1190–1201.

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FEATURE ARTICLE

Biology: an autonomous discipline

John R. Helliwell



A live (left) and cooked lobster.

Dame Ottoline Leyser, Professor of Plant Development at the University of Cambridge, UK, was quoted recently as saying “The defining feature of biology during the past few decades has been figuring out details of the parts. But biological systems don’t think they have parts” [1]. Scepticism of the role of reductionism in understanding biology is a theme in Ernst Mayr’s book *What Makes Biology Unique? Considerations on the Autonomy of a Scientific Discipline* [2]. Mayr even argues against the relevance of the discovery of the DNA double helix to understanding biology. Mayr, now 100 years old, retired from Harvard University in 1975, where he is now Emeritus Professor of Zoology. So, where do I think these strong views stand today against reductionist research, namely structural biology within which crystallography is a key player, as are the microscopies and spectroscopies? These latter two areas include cryoelectron microscopy (cryoEM) and nuclear magnetic resonance (NMR) spectroscopy. CryoEM in particular in recent years has taken the fight to these leading ‘whole biologists’ by opening up studies of large complexes that won’t crystallize yielding atomic details.

A thorny issue at its peak during the years of my graduate studies (1974 to 1977) was the relevance of the protein crystalline state to the solution state of a protein inside the biological cell. NMR provided atomically detailed results in solution and of course protein crystallography provided atomic details for a protein in the solid state. Studies of the structure and function of an enzyme in the crystalline state were to my mind greatly facilitated by the invention of the flow cell [3]. An example executing this to excellent effect was in the crystallographic studies of glycogen phosphorylase [4]. A pioneer in enzyme crystallography was David Blow and in his late-career overview [5] he lamented that a prediction of an

enzyme's reaction rate was still not possible, in effect defining it as one of today's continuing Grand Challenges for science. This seems a harsh assessment by David Blow to my view in that qualitatively one can now see directly for example that large substrate enzymes are much slower than small substrate enzymes. Furthermore, an enzyme's reaction rate can be deliberately slowed down, even stopped, by working with a designed mutant of the enzyme, guided by its 3D structure, again illustrating that, if not exactly a prediction of a specific reaction rate, this is a deliberate and successful alteration of enzyme reaction rate based on solid-state studies. Overall then crystallography has provided a powerful approach to this issue of the relevance of solid-state results with a resounding yes that these results are relevant to function; this important field has been reviewed by Keith Moffat [6]. These results overcame then the objections of the NMR solution-state spectroscopists to the crystallographer's results in the solid state. Weaknesses in the armoury of crystallography remain such as crystallization conditions, to a greater or lesser degree, taking one's results away from biological functioning conditions. Since those combative times in studies of protein structure, crystallography and NMR have worked in tandem to great effect in understanding structure and dynamics.

As protein crystallography has delivered ever more 3D structures, getting closer to complexity has proved a new challenge and focus. The accomplishments of virus crystallography and the crystal structure studies of the ribosome are testimony to the big steps forward to complexity yielding atomically detailed models of these molecular machines. The ribosome studies in particular required the perfecting of freezing conditions for the crystal so it would yield adequate amounts of X-ray diffraction data on the intense synchrotron beamlines needed to measure these data in a workable period of time.

A theme has steadily emerged in structural biology these last 20 years where there is a question about the strict relevance to biology of crystallography results now predominantly based on X-ray diffraction data measured at cryotemperature. This has been compounded by observations of specific X-ray damage to the crystallized protein. Conducting crystallography at physiological temperatures has then become an objective. Neutron macromolecular crystallography (nMX), whilst pursuing protein structures with protonation states experimentally determinable, has also automatically yielded room-temperature structures. Given also that projects succeed in getting time only where all other methods have failed, X-ray, electron or NMR based, it is clear that in structural biology there is a strategic importance of this method. nMX has seen a sustained growth of the instruments, the software and methods at leading neutron sources [7]. Furthermore, in an unconnected development, the new X-ray lasers yield X-ray diffraction data at room temperature and before radiation damage can kick in, the 'diffract before the sample is destroyed' approach [8]. Synchrotron facilities are now also adopting the X-ray laser methods for delivery of streams of micron-sized samples and thereby are also yielding results at physiological temperatures albeit not free of radiation damage like the X-ray lasers. To my mind an amazing accomplishment is the *room-temperature* crystal structure of the 30S ribosome using the Stanford LCLS [9]. The use of streams of micron-sized crystals raises the question of variations in those samples of the biological molecules being studied.

In making comparisons between a structure at cryotemperature and the same one at room temperature one has to be sure that each model refinement is at least at finality. The importance of refereeing of the underpinning data of a submitted article about a new crystal structure is to my mind paramount [10]. Even more, where comparisons between structures at two temperatures are concerned, then both should be refined to convergence. Validation of the structures of biological macromolecules is still developing [11].

In summary, the physical methods of crystallography, microscopy and spectroscopy continue to strive for, and do clearly deliver, biologically relevant results. Prediction of some aspects of biological function from atomic structure is possible, and that are also physiologically relevant. A founding father of quantum mechanics, the physicist Erwin Schrödinger posed the question *What is Life?* in his influential book [12]. It certainly influenced me as a young physicist looking towards what to pick as a research career. The fields of structural biology and crystallography have to my mind great contributions to make

in the future. Shall we ever convince 'whole biology biologists'? Time will tell but it is unlikely to be in my lifetime. In one of my own research themes studying the basis of the coloration of the lobster shell our explanations cover the molecular basis of the coloration [13, 14] but of course not why the lobster has that colour for its shell. One could say that our research on that is only 'skin deep'.



Lobsters caught by fisherman at the Isle of Whithorn, Scotland. [Author's own photograph.]

References

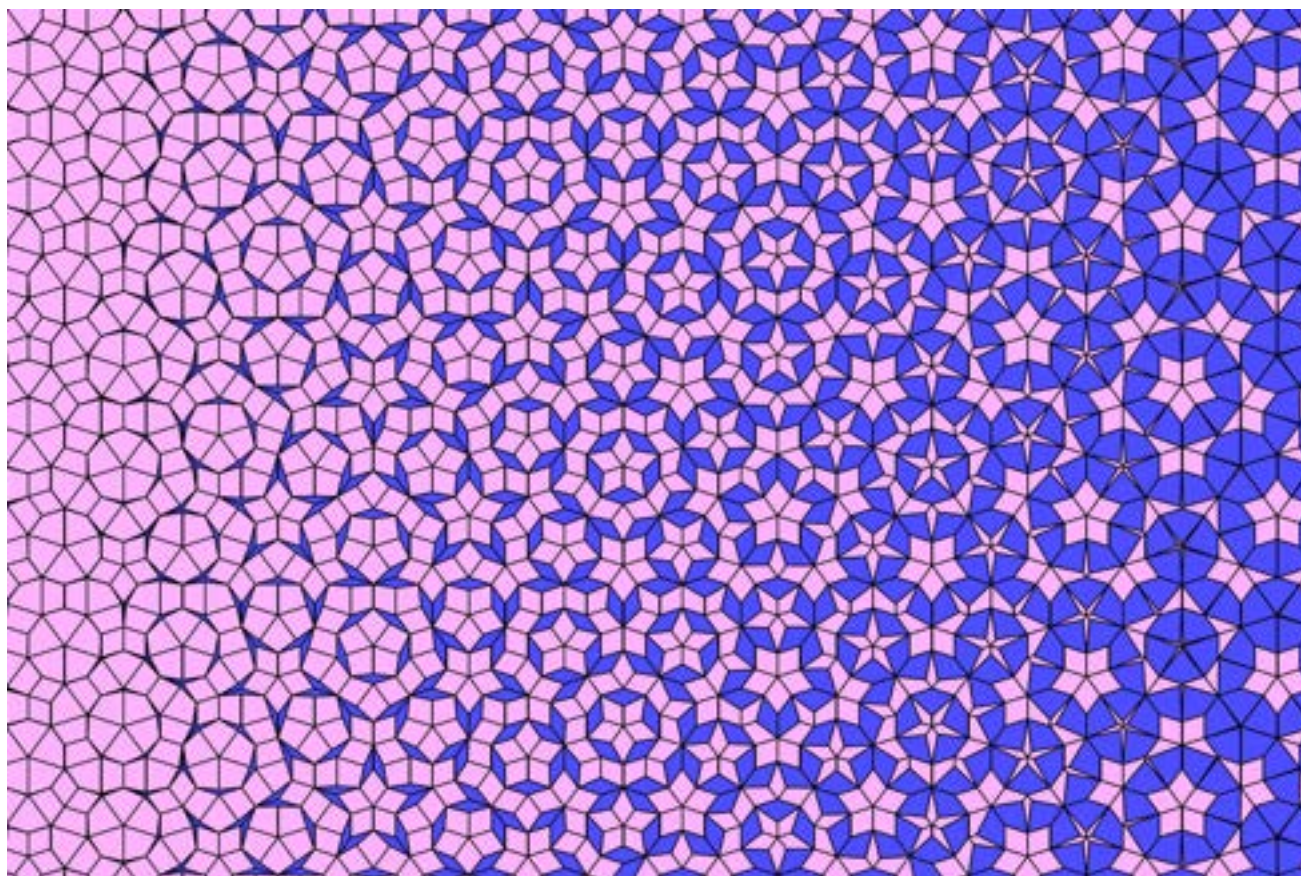
- [1] Turney, J. (2019). The puzzle of life. *Times Higher Education*, 21 February 2019, pp. 44–45.
- [2] Mayr, E. (2004). *What Makes Biology Unique? Considerations on the Autonomy of a Scientific Discipline*. Cambridge: Cambridge University Press.
- [3] Wyckoff, H. W., Doscher, M., Tsernoglou, D., Inagami, T., Johnson, L. N., Hardman, K. D., Allewell, N. M., Kelly, D. M. & Richards, F. M. (1967). Design of a diffractometer and flow cell system for X-ray analysis of crystalline proteins with applications to the crystal chemistry of ribonuclease-S. *J. Mol. Biol.* **27**, 563–578.
- [4] Hajdu, J., Acharya, K. R., Stuart, D. I., McLaughlin, P. J., Barford, D., Oikonomakos, N. G., Klein, H. & Johnson, L. N. (1987). Catalysis in the crystal: synchrotron radiation studies with glycogenphosphorylase b. *EMBO J.* **6**, 539–546.
- [5] Blow, D. M. (2000). So do we understand how enzymes work? *Structure*, **8**, R77–R81.
- [6] Moffat, K. (2001). Time-Resolved Biochemical Crystallography: A Mechanistic Perspective. *Chem. Rev.* **101**, 1569–1581.
- [7] Blakeley, M. P. & Podjarny, A. D. (2018). Neutron macromolecular crystallography. *Emerg. Top. Life Sci.* **2**, 39–55.
- [8] Neutze, R., Wouts, R., van der Spoel, D., Weckert, E. & Hajdu, J. (2000). Potential for biomolecular imaging with femtosecond X-ray pulses. *Nature*, **406**, 752–757.

- [9] Dao, E. H., Poitevin, F., Sierra, R. G., Gati, C., Rao, Y., Ciftci, H. I., Akşit, F., McGurk, A., Obrinski, T., Mgbam, P., Hayes, B., De Lichtenberg, C., Pardo-Avila, F., Corsepilus, N., Zhang, L., Seaberg, M. H., Hunter, M. S., Liang, M., Koglin, J. E., Wakatsuki, S. & Demirci, H. (2018). Structure of the 30S ribosomal decoding complex at ambient temperature. *RNA*, **24**, 1667–1676.
- [10] Helliwell, J. R. (2018). Data science skills for referees: I biological X-ray crystallography. *Cryst. Rev.* **24**, 263–272.
- [11] Helliwell, J. R. (2017). New developments in crystallography: exploring its methods, technology and scope in the molecular biosciences. *Biosci. Rep.* **37**, BSR20170204.
- [12] Schrödinger, E. (1943). *What is Life? The Physical Aspect of the Living Cell*. Based on lectures delivered under the auspices of the Dublin Institute for Advanced Studies at Trinity College, Dublin, in February 1943. Reprinted by Cambridge University Press, 2012.
- [13] Cianci, M., Rizkallah, P. J., Olczak, A., Raftery, J., Chayen, N. E., Zagalsky, P. F. & Helliwell, J. R. (2002). The molecular basis of the coloration mechanism in lobster shell: β -crustacyanin at 3.2 Å resolution. *Proc. Natl Acad. Sci. USA*, **99**, 9795–9800.
- [14] Rhys, N. H., Wang, M.-C., Jowitt, T. A., Helliwell, J. R., Grossmann, J. G. & Baldock, C. (2011). Deriving the ultrastructure of α -crustacyanin using lower-resolution structural and biophysical methods. *J. Synchrotron Rad.* **18**, 79–83.

FEATURE ARTICLE

Deformed Penrose tiling and quasicrystals

Richard Welberry



One of the most remarkable developments in crystallography during the years in which I have been active in the field was the discovery in 1984 (Shechtman *et al.*, 1984) of quasicrystals — materials displaying symmetries forbidden in classical crystallography. Given that the concepts of classical crystallography had held precedence for the best part of a century, not only was it remarkable that such materials could exist but also was it perhaps more remarkable that in diffraction experiments they produced Bragg-like peaks comparable in sharpness to those from ordinary crystals. Since their discovery these novel materials have been the subject of intense study by experimental and theoretical scientists, and a whole new field has emerged.

Although this new field was rather removed from the path that had already been set for my own research – namely single-crystal diffuse scattering and disorder – I was instantly entranced by the new discoveries and felt compelled to become involved in some way. I was particularly captivated by the tiling models, such as Penrose tiling (Penrose, 1974), that were used to aid the understanding of quasicrystalline structure. Such tilings provide an attractively simple conceptual extension of conventional crystallography. Instead of the normal repeating “unit cell” of a crystal there are now two different “tiles” (e.g. a fat and a thin rhombus in 2D), each of which can be decorated by an arrangement of atoms. In addition, I found the tiling patterns themselves aesthetically very appealing.

The “matching rules”, which define the ways tiles can be assembled to form the Penrose pattern, ensure that the structure is coherent and locally consistent across tile boundaries. Unfortunately, real quasicrystals do not correspond exactly to this tiling picture, although the correspondence may

sometimes be quite close. A tiling model may give sharp Bragg reflections at points corresponding to the observed quasicrystal diffraction peak *positions*, but it is not possible to decorate the two types of tiles in a way that reproduces the observed Bragg peak *intensities* (Steurer, 2004). The tiling analogy has nevertheless remained useful in exploring many other aspects of quasicrystals and their relationship to normal crystals.

One area that I found of particular interest was that the basic Penrose pattern could be subject to local *deformations* rather akin to the local “size-effect” distortions that have played an important role in many of our studies of diffuse scattering in crystals. These deformations in quasicrystals may be described in terms of mathematical constructions called “deformed model sets” (Hof, 1997; Bernuau & Duneau, 2000; Baake & Sing, 2004; Baake & Lenz, 2005; Sing & Welberry, 2006). Examples of deformed model sets may be constructed by simple prescription and contain no randomness. They give diffraction patterns that have sharp Bragg peaks and no diffuse scattering. Nevertheless both the tiling pattern and its diffraction pattern may be very different from the original undeformed pattern. Such constructions lead to many new, interesting and aesthetically pleasing patterns.

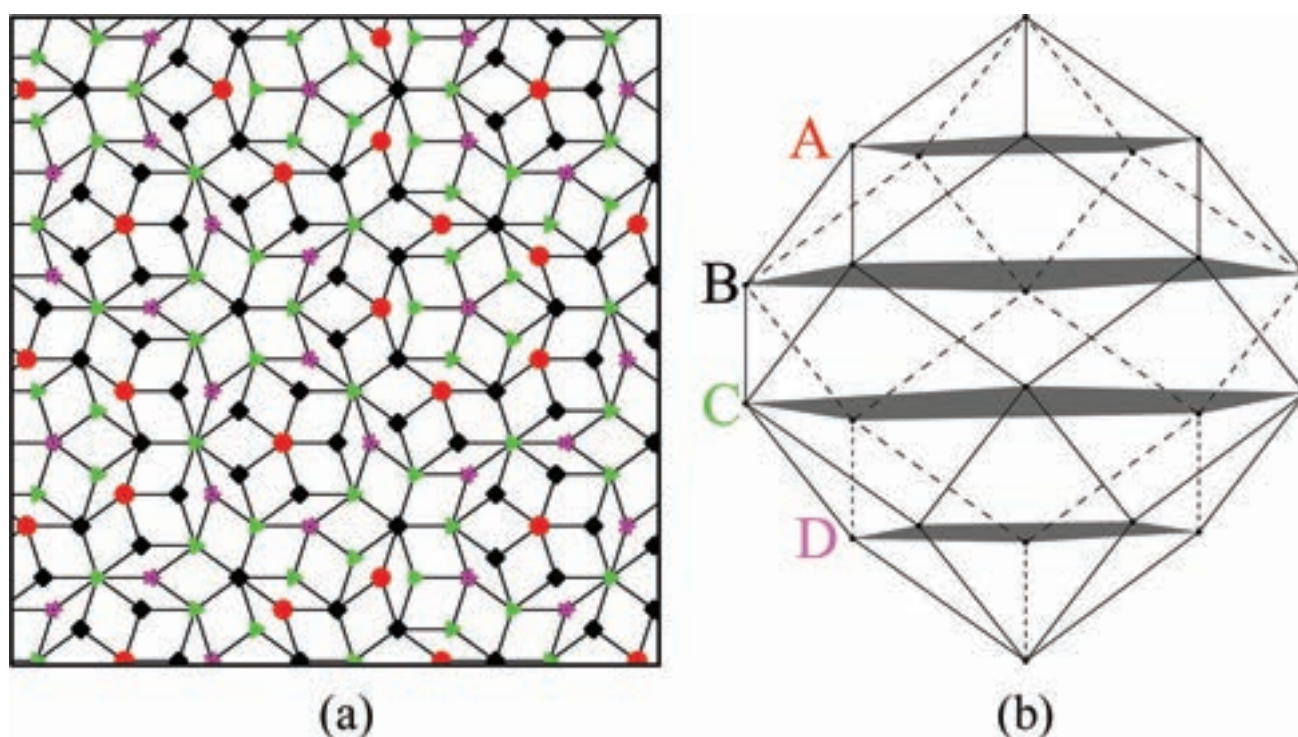


Figure 1. (a) Small region of Penrose tiling showing the four different kinds of vertex [circle (red), square (black), triangle (green) and star (pink)]. (b) The rhombicosahedron internal space projection window showing the four planes (A, B, C and D) from which the different vertices derive.

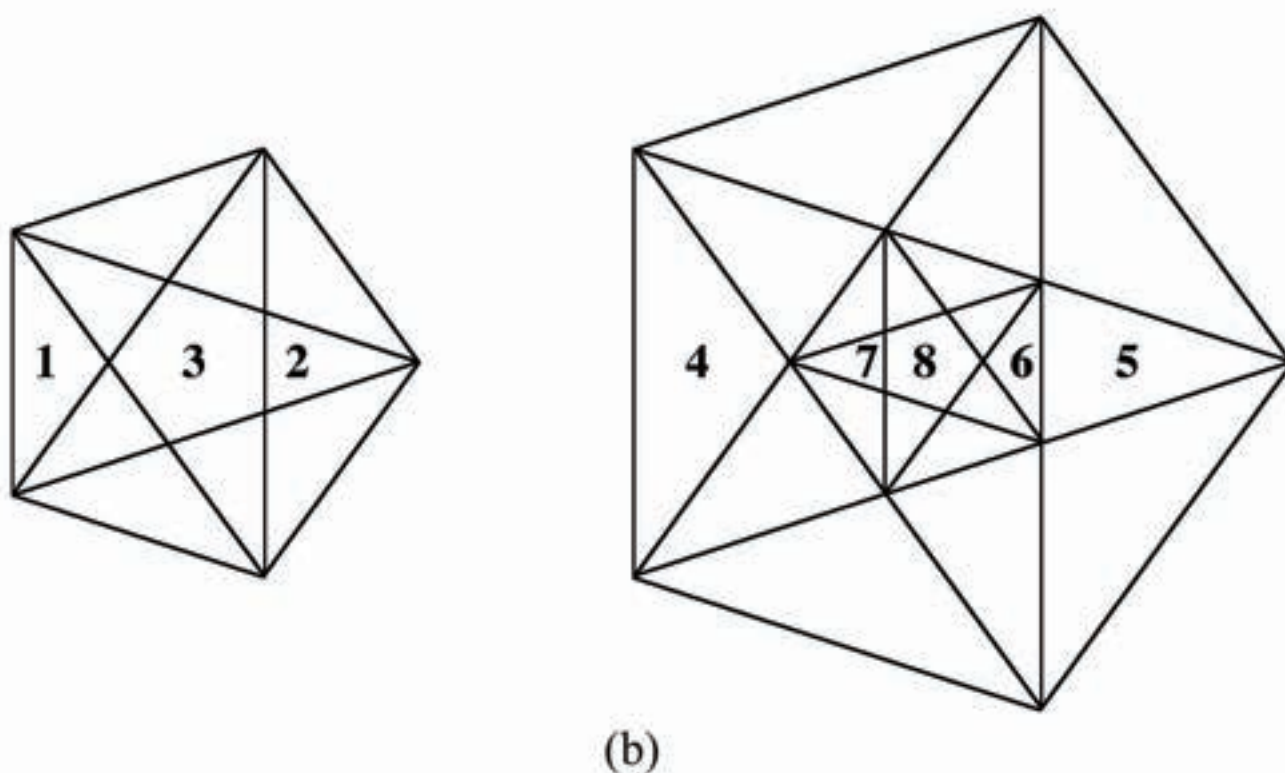
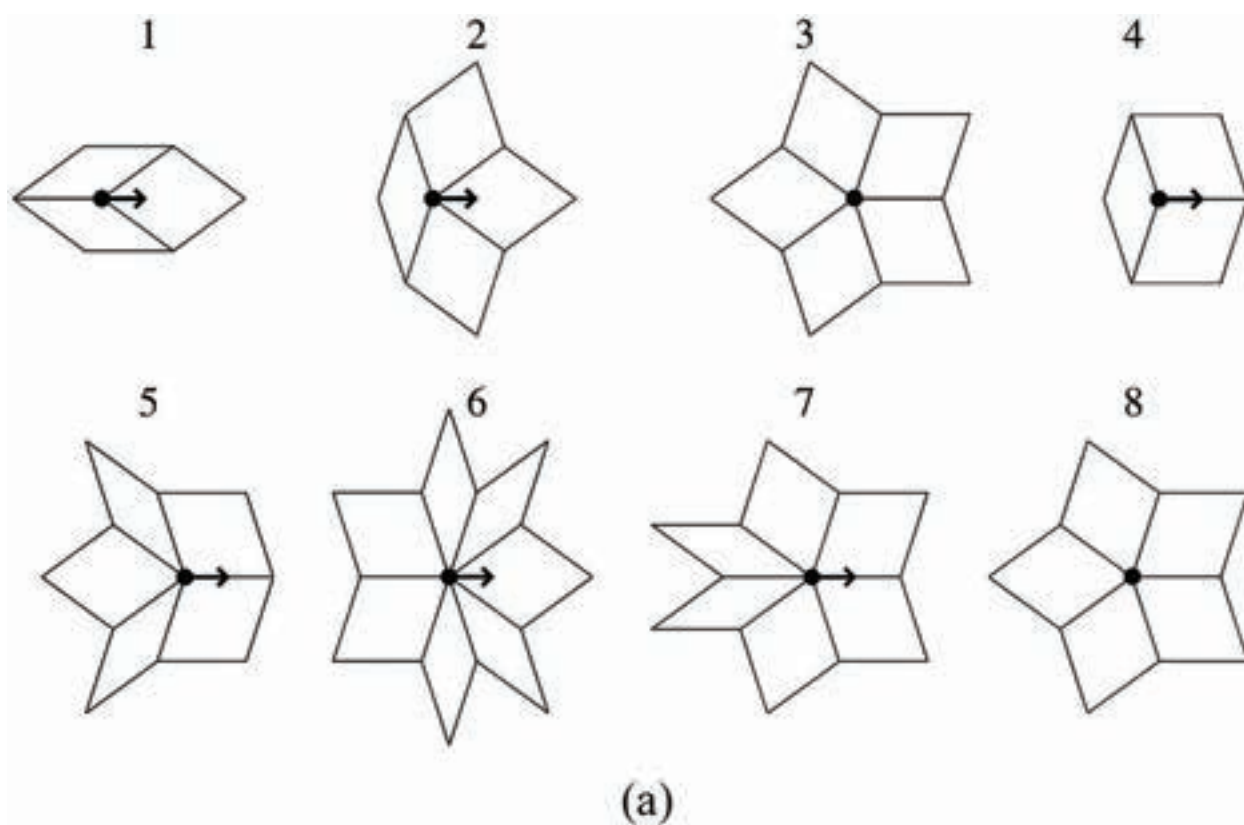


Figure 2. (a) Different types of tile cluster. Arrows represent the displacement vectors v_1 , v_2 , v_4 , v_5 , v_6 and v_7 (see text). (b) The small (A and D) and large (B and C) pentagonal sections from the projection volume showing the subregions that give rise to the eight different types of cluster shown in (a). Clusters 1 to 3 derive from A and D while 4 to 8 derive from B and C.

Construction of deformed Penrose tiling patterns

2D Penrose rhomb tiling may be obtained by projection from 5D hypercubic space following the method described by Yamamoto & Ishihara (1988). A small region of this tiling is shown in Fig. 1a. Using this projection method, each vertex of the 2D tiling pattern (in the physical space) derives from a point within the 3D projection window (in the internal space). Here, the projection window is the rhombic icosahedron (Fig. 1b) and the four different types of vertex (circle, square, triangle and star) derive from points that lie in the four (shaded) pentagon-shaped plane sections A, B, C and D. If the local environment of any given vertex is considered, it is found that there are eight different kinds of configuration (clusters) possible (each with its symmetry equivalents) (Fig. 2a). Each of these cluster types derives from a point lying in a given subregion of the projection pentagons. Fig. 2b shows the different subregions that give rise to the different cluster types.

The Penrose tiling pattern that is obtained by the projection method can be deformed in such a way that it remains pure point diffractive. Each vertex in real (physical) space is displaced from its ideal position by an amount v_i in a direction ϕ_i where v_i and ϕ_i are given by a function defined in the internal space window. We use a simple function in which it is assumed that v_i and ϕ_i are constant over the area of each subregion of the two pentagons shown in Fig. 2b. It is assumed that the direction $\phi_i = 0$ corresponds to the direction drawn in each cluster figure of Fig. 2a and rotates with each symmetry equivalent cluster to remain along the mirror plane of the cluster. The six different v_i corresponding to regions 1, 2, 4, 5, 6 and 7 may each be chosen independently but it is assumed that symmetry-equivalent regions have identical values, ensuring overall symmetry is maintained. As a displacement of vertex 3 or 8 would break local symmetry it is assumed that $v_3 = v_8 = 0$.

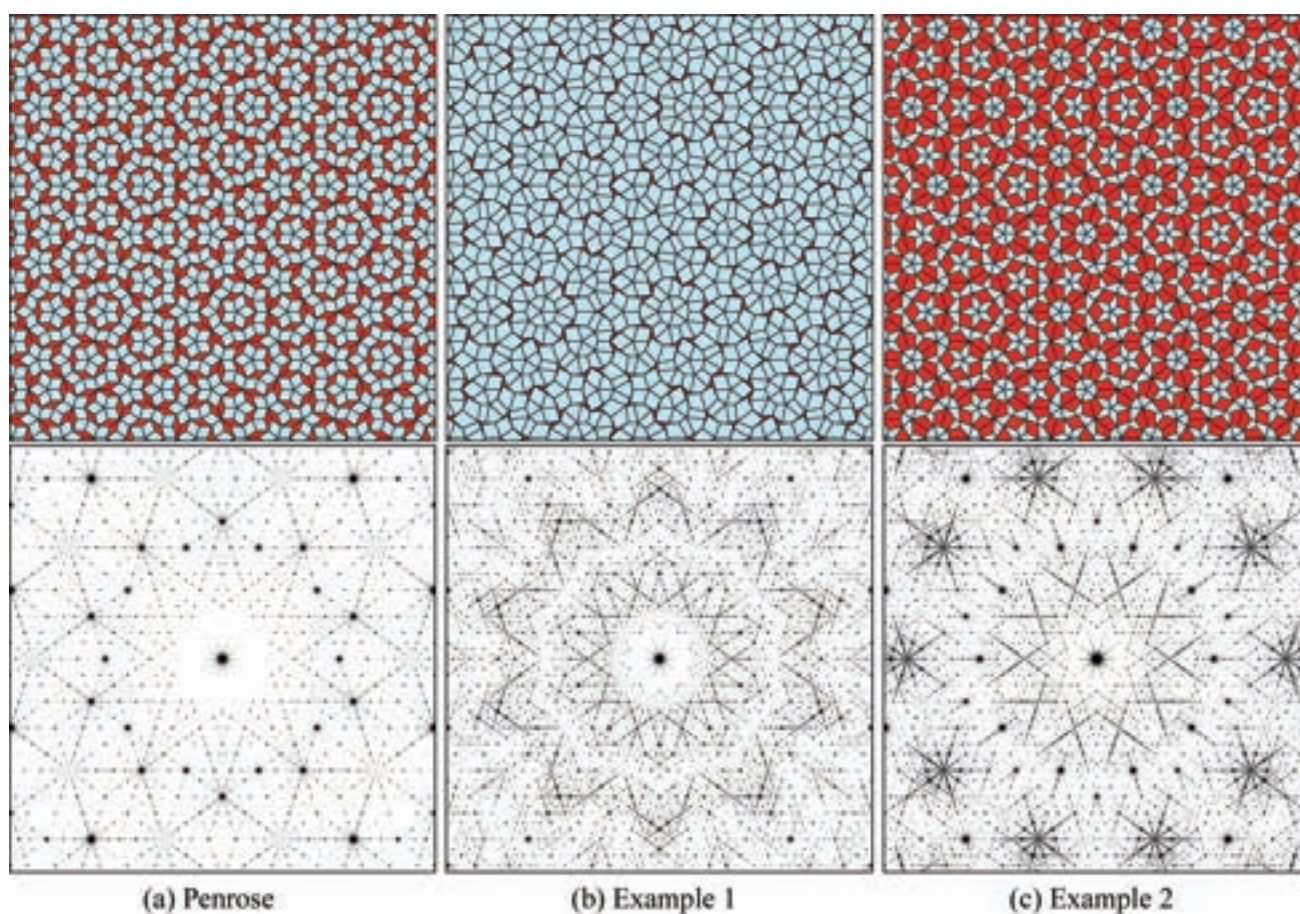


Figure 3. Regions of (a) undeformed Penrose tiling and (b) and (c) deformed tilings, together with their computed diffraction patterns. Remarkably, all three of these diffraction patterns have the same Bragg peak positions yet extremely different intensity distributions – and none of them show diffuse scattering.

Despite the simplicity of the deformation function defined above there are 12 parameters that may be chosen independently: $\nu_1, \nu_2, \nu_4, \nu_5, \nu_6, \nu_7$ and $\phi_1, \phi_2, \phi_4, \phi_5, \phi_6, \phi_7$, each representing a displacement magnitude or a displacement direction for one of the non-fivefold symmetric cluster types (Fig. 2). We present here just two contrasting examples to show how the deformation works. Quite large values of the displacements have been used to produce the most striking visual effects but it should be remembered that a continuous range of values is possible from the Penrose pattern for which all displacement parameters are zero (Fig. 3a) through to these more extreme cases. The magnitudes of the displacements given are on a scale for which the edge length for the Penrose rhombs was $1/\tau$ Å where $\tau \approx 1.618$ is the golden ratio.

Example 1. $\nu_1 = \nu_2 = \nu_4 = \nu_5 = \nu_6 = \nu_7 = -0.4$; all $\phi_i = 0.0$. The results for this set of parameters are shown in Fig. 3b. Reference to Fig. 2a shows that setting all the displacements to be negative “closes up” what were thin rhombs while in the main enlarges what were fat rhombs. The real space pattern thus has a predominance of the blue (light) colour, with a small amount of red (dark) in the interstices. Instead of only two shapes for the original tiles the pattern is now composed of a multitude of different shapes and sizes more like cobblestones than tiles. Despite this seeming randomness the diffraction pattern still consists only of Bragg peaks, though with drastically altered intensities.

Example 2. $\nu_1 = 0.8$; $\nu_2 = \nu_4 = 0.4$; $\nu_5 = \nu_6 = \nu_7 = 0.0$; all $\phi_i = 0.0$. The results for this set of parameters are shown in Fig. 3c. Now many of the original thin rhombs have been expanded giving a predominant overall red colour. These particular values were chosen in order to give some clusters the appearance of a blue five-pointed star in a red pentagon. Again the pattern is made up of a multitude of different shapes and sizes but again the diffraction pattern consists only of Bragg peaks and again has drastically altered intensities.

Tiling with variable deformation

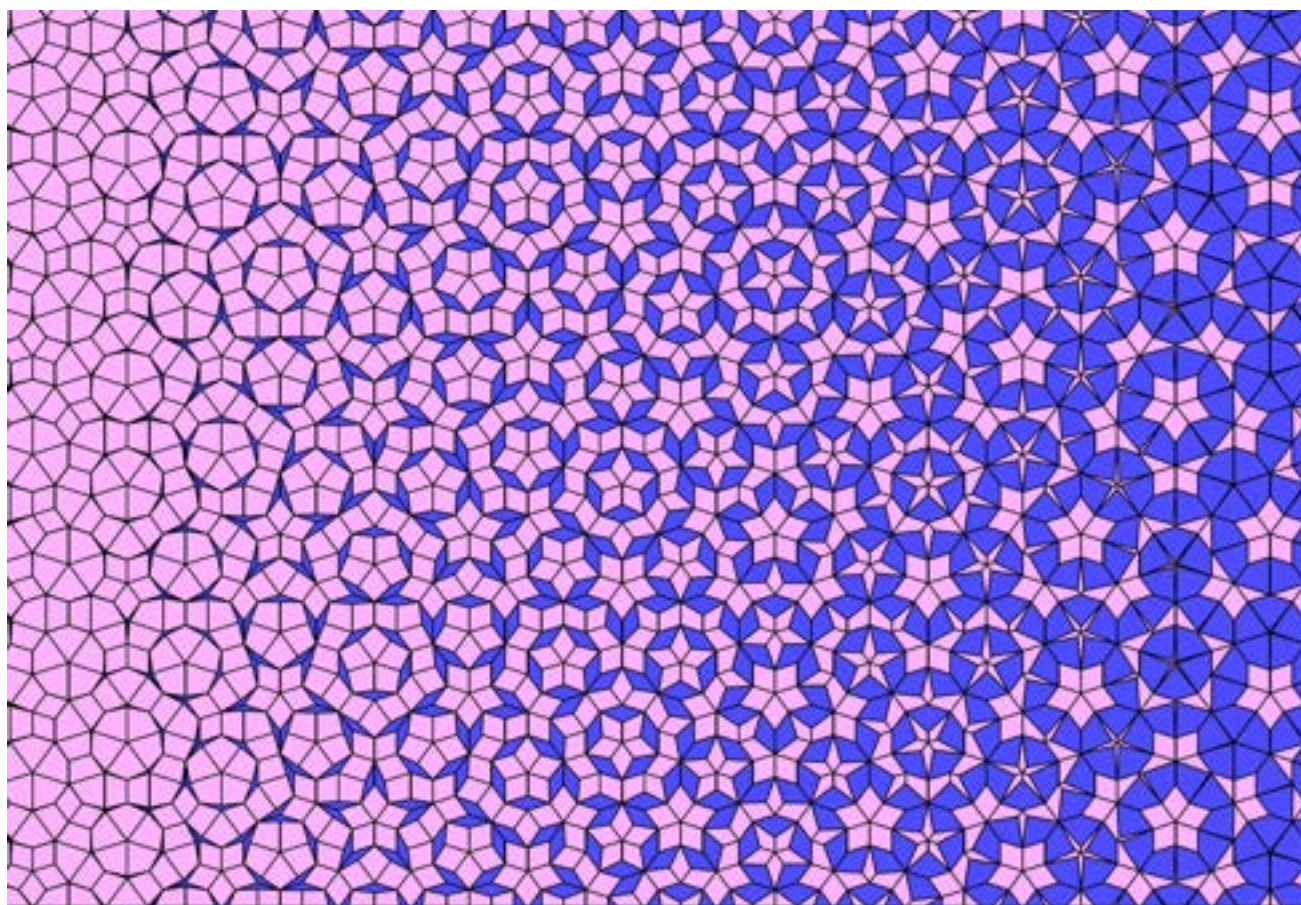


Figure 4. A tiling pattern in which the deformation parameters have been varied linearly from left to right.

Fig. 4 shows a pattern that has been produced by deforming a Penrose tiling using two sets of v_i, ϕ_i parameters. At each horizontal position the value of the parameters is a linear combination of those that produce the pattern at the left extreme to those that produce the pattern at the right. In the middle the displacement parameters are zero and the pattern is the undeformed Penrose tiling. On the left the fat rhombs have been expanded, making the pattern appear predominantly pink while on the right the thin rhombs have expanded, making the pattern appear predominantly blue. This is my favourite pattern and one that I use in my Macintosh screensaver using the algorithm called “Origami” (see video).

In producing this pattern I admit to receiving inspiration from some of the drawings of M. C. Escher.

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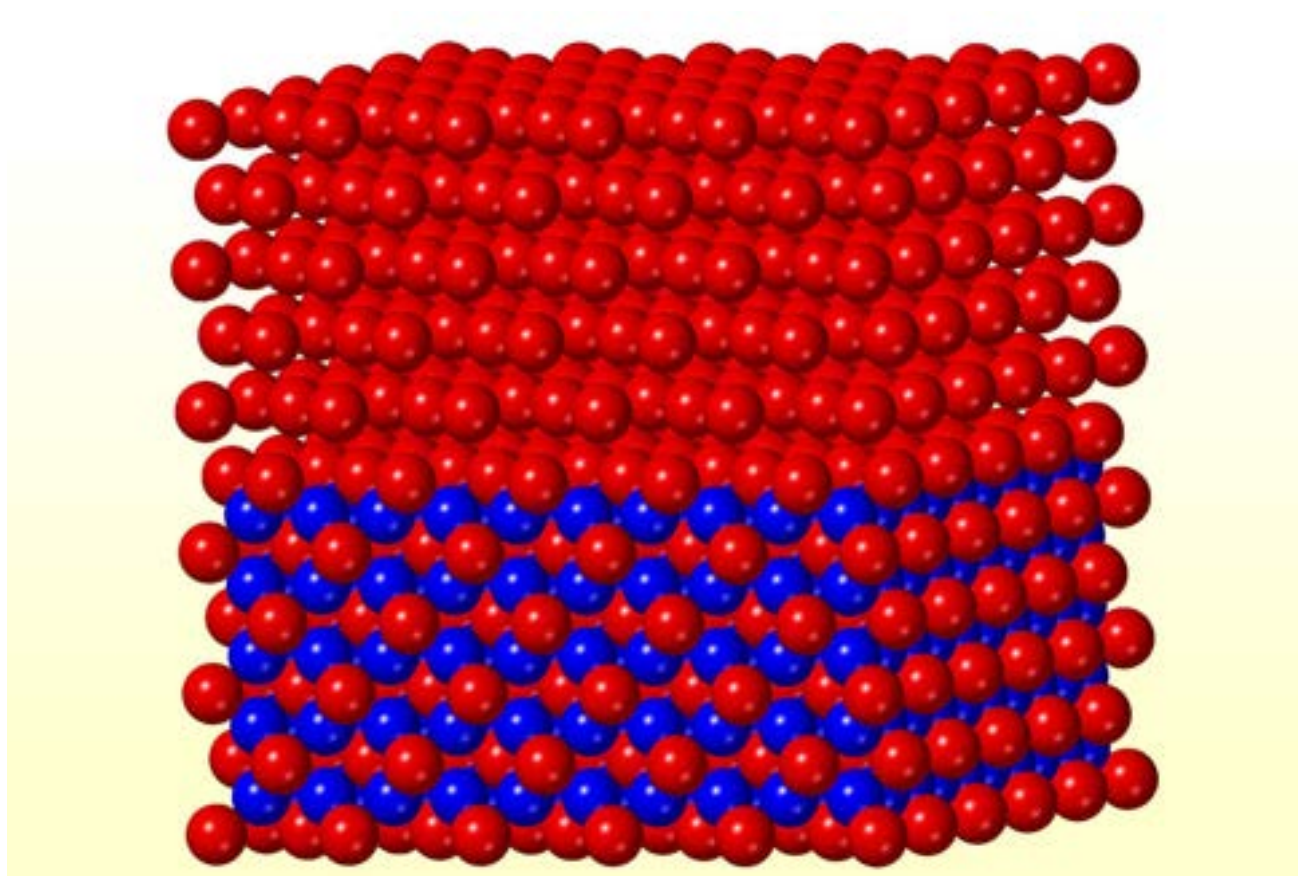
References

- Baake, M. & Lenz, D. (2005). *J. Fourier Anal. Appl.* **11**, 125–150.
- Baake, M. & Sing, B. (2004). *Canad. Math. Bull.* **47**, 168–190.
- Bernuau, G. & Duneau, M. (2000). *Directions in Mathematical Quasicrystals*, edited by M. Baake & R. Moody, CRM Monograph Series, **13**, 43–60. Providence, Rhode Island: AMS.
- Hof, A. (1997). In *The Mathematics of Long-Range Aperiodic Order*, edited by R. Moody, pp. 239–268. Dordrecht: Kluwer Academic Publishers.
- Penrose, R. (1974). *J. Inst. Math. Appl.* **10**, 266–271.
- Shechtman, D., Blech, I., Gratias, D. & Cahn, J. (1984). *Phys. Rev. Lett.* **53**, 1951–1953.
- Sing, B. & Welberry, T. R. (2006). *Z. Kristallogr.* **221**, 621–634.
- Steurer, W. (2004). *Z. Kristallogr.* **219**, 391–446.
- Yamamoto, A. & Ishihara, K. (1988). *Acta Cryst.* **A44**, 707–714.

FEATURE ARTICLE

The super-sub schizophrenia

Massimo Nespolo



In the previous issue of the *IUCr Newsletter*, I drew the reader's attention to [the difference between a crystal structure and its \(Bravais\) lattice](#). This was needed because of the surprisingly widespread misunderstanding that shows up in so many textbooks, articles and lectures. This time we dig a little deeper and try to see what happens when “something” is added to or removed from, in a systematic way, a lattice and a structure.

First of all, let us consider a lattice, *i.e.* the mathematical abstraction made up of zero-dimensional points (the lattice nodes) that represents the periodicity of a crystal structure (remember, there are no atoms in a lattice). To a lattice, one can only add lattice nodes; similarly, from a lattice, one can only remove lattice nodes. This may at first just seem a mind game but we are going to see its physical meaning.

What does it mean to add to a lattice (let us call it L1 for simplicity) a set of nodes so that one obtains another lattice (let us call it L2)? If you choose one lattice node as the origin (it does not matter which you choose, they are all equivalent), then you can draw an infinite set of vectors from that origin to all the other lattice nodes. Each of these vectors represents a translation operation and all these translations do form a mathematical group: the translation group of L1 (which is a subgroup of the space group of the structure whose lattice is L1). When you add lattice nodes, you add further vectors, *i.e.* further translation operations. These, together with the translations of L1, again form a group and, because the order of the group (number of operations) has increased, it is actually a supergroup of that of L1. It should therefore come as no surprise that L2 is a *superlattice* of L1.

Now, let us think about the unit cells of the two lattices, and in particular the primitive unit cells. Because of the additional nodes in L2 with respect to L1, the primitive unit cell of L2 is smaller than the primitive unit cell of L1 and is therefore a subcell (Figure 1). So, we get the surprising result that the primitive unit cell of the superlattice is a subcell of that of the original lattice.

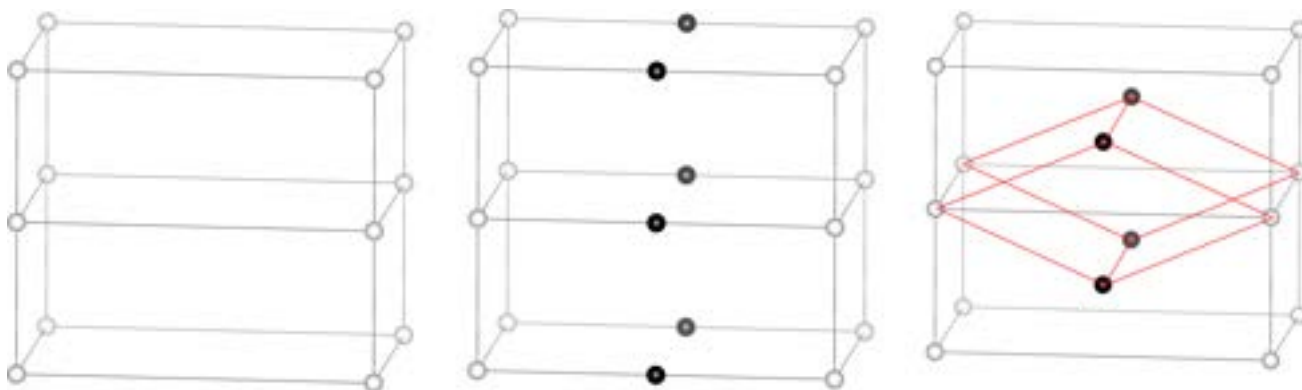


Figure 1. Primitive unit cell of the original lattice L1 (left) and of two superlattices L2 obtained by adding a second (infinite) set of lattice nodes (black) obtained from the original by translations $0, \frac{1}{2}, 0$ (middle) and $0, \frac{1}{2}, \frac{1}{2}$ (right). Axes: a is towards the observer, b is horizontal and c is vertical. The figure shows two unit cells of L1 along the c axis. The primitive unit of the superlattice in the middle has its edges parallel to that of L1 but its translation vector along b is half of that of L1. The primitive unit cell of the superlattice on the right is outlined in red.

Let us next do the opposite: remove a subset of lattice nodes from L1 so that the remaining lattice nodes still form a lattice L2. The set of translation vectors of L2 is a subset of that of L1; therefore, the group of translations of L2 is a subgroup of the group of translations of L1. As a consequence, L2 is a *sublattice* of L1, whereas its primitive unit cell is a *supercell* of that of L1 (Figure 1 applies again, this time by considering the middle and right parts as representing L1, the left part representing L2). So now we learn that a *sublattice* consists of *supercells*.

In the literature, this simple relation is quite often misunderstood. If the primitive unit cell of L2 is larger than that of L1, *i.e.* if it is a supercell, then L2 is itself often, but incorrectly, called a “superlattice”; it is actually a sublattice, because it has lost symmetry operations (in particular, translations) with respect to L1. Quite obviously the relation sub–super is reversed in going from one space to its dual (direct $\leftrightarrow$ reciprocal). A simple graphic guide to avoid this type of mistake is provided in Figure 2.

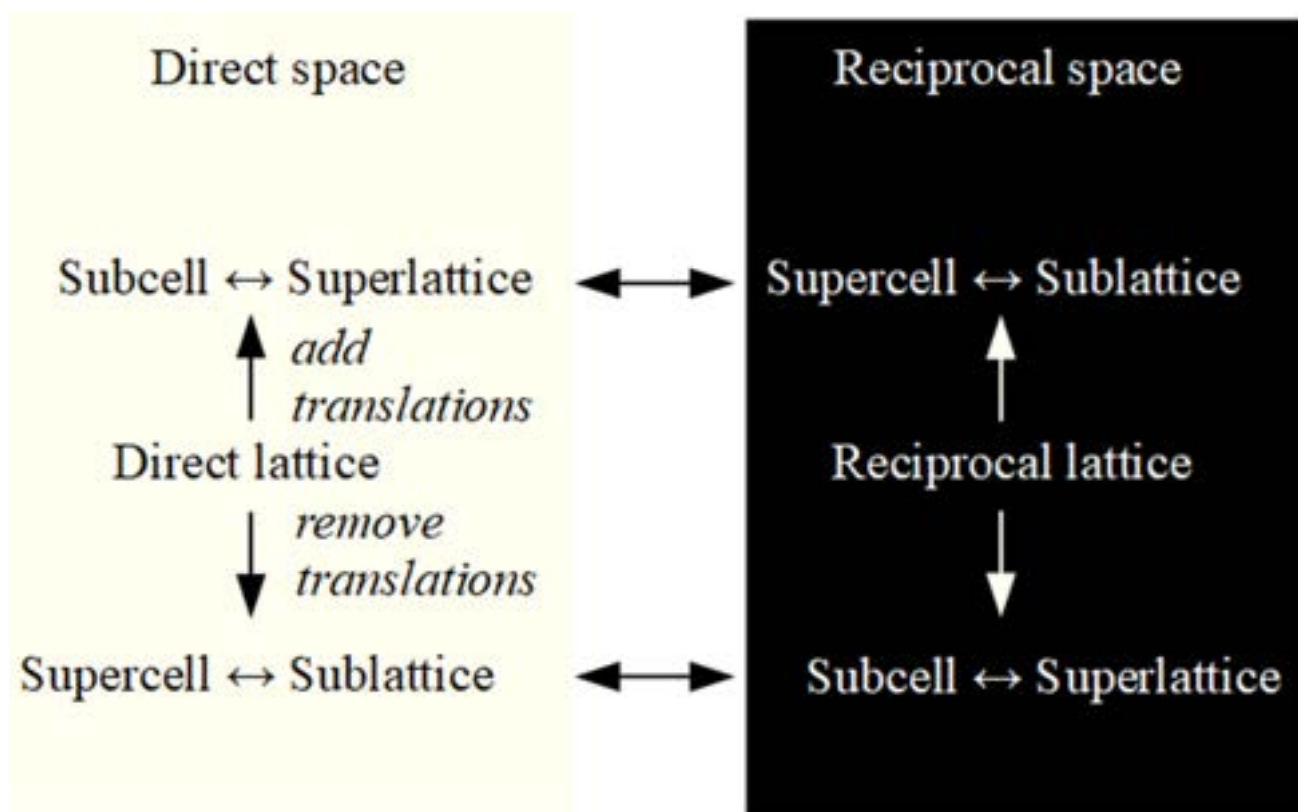


Figure 2. The relation between a lattice and its super/sublattices in the dual spaces.

When one sees extra diffraction spots (“extra” with respect to what one expects to see...) in the diffraction pattern, one speaks of *superlattice diffractions*, which is perfectly consistent, considering that the periodicity in the reciprocal lattice has increased. However, the crystal structure that has caused these extra diffractions corresponds to a *sublattice* in direct space. So, when talking about diffraction (reflections, peaks) one uses the super-sub terminology for reciprocal lattices rather than for direct lattices.

Let us now move to the structure (built by atoms) and analyse the meaning of superstructure and substructure.

In a crystal structure some atomic positions may statistically be occupied by different types of atoms (let us say two, for the sake of simplicity). This often occurs in inorganic and mineral structures, where atoms are disordered at positions that are equivalent under the operations of the space group. Under some changes of the external conditions (temperature, pressure, applied field, etc.) the disorder distribution may no longer be stable and a phase transition may occur, after which different atoms become ordered. The structure with a disordered atomic distribution is called a *basic structure*. The positions that were equivalent before the transition are no longer equivalent afterwards. Depending on whether the ordering does or does not involve a reduction in the translational symmetry (*i.e.* whether or not the primitive unit cell is transformed to a supercell), the resulting structure is called a *superstructure* or a *derivative structure* (Figure 3). Note that, because the unit cell of the superstructure is a *supercell* of the unit cell of the basic structure, its lattice is actually a *sublattice* of that of the basic structure!

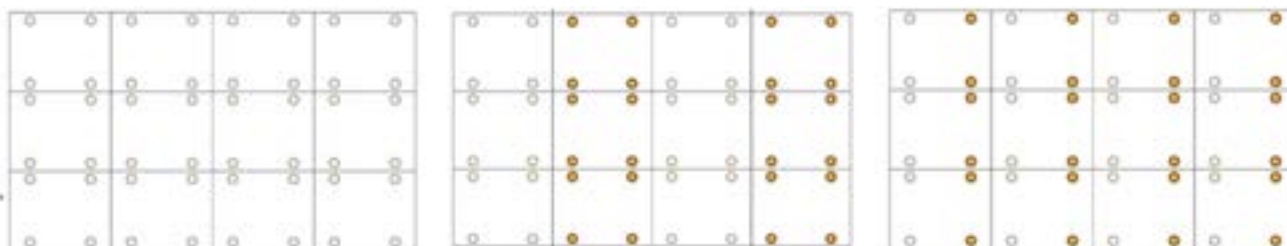


Figure 3. A simple example of a basic structure (left), superstructure (middle) and derivative structure (right).

The term superstructure is also used in a different, although not unrelated, meaning when studying modular structures. A crystal structure is built by the periodic and regular repetition of a structural element: a molecule (in the case of molecular crystals), a set of atoms or ions forming a coordination polyhedron (in the case of a non-molecular crystal, e.g. NaCl) or an extended network (like in the case of metals). In some cases, one can ideally cut the crystal structure into bigger and more complex building blocks: layers (sheets), rods (chains) or finite modules composed of a number of atoms significantly larger than those identifying a coordination polyhedron. These crystals are known as modular structures, and can be seen as *superstructures* with respect to the modules. Here another common mistake must be pointed out. The modules are subperiodic, i.e. they are periodic in a subspace of three-dimensional space (diperiodic, monopericodic or nonperiodic depending on whether the module is a layer, a rod or a finite block) but they are not “low-dimensional”. The expression “low-dimensional material” that today pollutes scientific literature is a semantic nonsense.

The last concept to consider is the *substructure*. A crystal structure is composed of $N \geq 1$ atoms in the asymmetric unit and all those equivalent, obtained by applying the symmetry operations of the space group. Stated in an equivalent and more general way, remembering that the infinite set of atoms equivalent under the action of the space group is called a *crystallographic orbit*, a crystal structure is composed of $N \geq 1$ crystallographic orbits. When $N > 1$, one can consider a subset M ($1 \leq M < N$) of the crystallographic orbits, and obtain, in this way, a *substructure*. Now, when one considers only the periodicity of a substructure, one gets the lattice of this substructure. Its unit cell can either coincide with that of the whole structure or be a *subcell*. Therefore, the lattice of a substructure either coincides with the lattice of the original structure or is a *superlattice* of it: it can never be a sublattice. Despite the fact that these concepts and definitions sound crystal (!) clear, many publications call a substructure “sublattice”, which not only is plain wrong even when considering the lattice of the substructure, but also shows, once more, the deep-rooted confusion between structure and lattice that we analysed in the last contribution. Here is [one recent example](#), but one can easily find a lot more by a simple keyword search on the World Wide Web. It is to be emphasized that this sloppy language is quite common in high-impact journals, such as in the example above: impact factors are by no means a guarantee of sound science. [IUCr journals](#) of course do not fall into this sort of trap!

I conclude this short survey by pointing out that is not uncommon to find serious mistakes occurring even in official definitions provided by non-specialists. For example, the entry *superlattice* in the *IUPAC Gold Book* represents a double mistake: because it actually deals with the concept of **superstructure** and because the lattice of this superstructure is a **sublattice**. It is to be noted that the same *IUPAC Gold Book* does not have any entry for “sublattice”, “superstructure” or “substructure”. It is highly regrettable that societies in other fields take the initiative of providing definitions without checking whether they are correct with the specialists. We can only hope that in the future they will check with the reference for crystallographic terms, which is the [Online Dictionary of Crystallography](#).

References

Buerger, M. J. (1947). *J. Chem. Phys.* **15**, 1–16.

Ferraris, G., Makovicky, E. & Merlino, S. (2008). *Crystallography of Modular Materials*, 2nd ed., p. 384. Oxford University Press.

Nespolo, M. (2019). *J. Appl. Cryst.* **52**, 451–456.

IUCR CONGRESS

Preparation and promotion of the 25th IUCr Congress in Prague, Czech Republic

Radomír Kužellvna Kutá Smatanová



Český Krumlov in South Bohemia, site of one of the post-Congress trips.

Once the list of all plenary and keynote speakers had been accepted by the IUCr Executive Committee in June 2019, we started to send invitation emails from programme@iucr2020.org. In many cases more attempts were necessary and sometimes different addresses had to be used because of spam filters, which can block such general conference addresses. After two and half months of communications, all plenary and keynote lectures now have been confirmed. With respect to the original proposals from the May 2019 International Programme Committee meeting we have made only one change and applied one alternative for the same topics. We are proud to announce a plenary talk by the 2016 Nobel Prize in Chemistry winner Sir Francis Stoddart on "How crystallography helped to create a new bond in chemistry". We also look forward to plenary lectures from Helen Berman on "How data have revealed the structural universe" and David Eisenberg on "The structural biology of pathogenic amyloid fibrils".

A total of 36 keynote lectures will be presented, 3 in parallel in 12 blocks at the beginning and end of each conference day. The keynote speakers with their photos can be seen [here](#). One of the keynote lectures is devoted to the winners of the Gjønnnes Medal in Electron Crystallography, Sven Hovmöller and Ute Kolb.

Currently, we have 137 confirmed co-chairs out of a total number of 208 persons for 104 regular sessions.

Satellites and workshops are under discussion. In collaboration with some IUCr Commissions and others we are planning the following:

- Computing school, 17–22 August in Nové Hradky, South Bohemia
- Electron crystallography school, 19–22 August in Tábor, South Bohemia
- Small-angle scattering workshop, 19–21 August in Prague
- Macromolecular Machines in Biomedicine: Structure, Dynamics, and Evolution workshop, 21–22 August at the Prague Congress Centre
- New trends in solution and refinement of aperiodic and magnetic structures workshop, 21–22 August in Prague
- ICDD workshop, 22 August at the Prague Congress Centre.



International Tables Volume H Editor Jim Kaduk (left) and IUCr Executive Managing Editor Peter Strickland in discussion at the joint IUCr/Congress booth at ACA2019.

We have also been working hard to promote the Congress. We shared a booth with the IUCr at the APS (American Physical Society) March Meeting 2019 in Boston, MA, USA, which hosted nearly 12,000 participants, and did the same at the ACA meeting in Covington, KY, USA, in July 2019. In order to attract more people, we ran a competition for a free registration to the Congress (other prizes were a 50% discount and a free ticket for the conference dinner). Unfortunately, the next ACA meeting is scheduled for 2020 in San Diego, CA, USA, about two weeks before the Prague Congress, so it may be inconvenient for people to attend both conferences. Of course, we were also present at ECM32 in Vienna, Austria, where we shared a booth with the German Crystallographic Society, which is going to bid for IUCr2029 in Berlin. In addition to posters and promotion materials we also served Pilsner beer. We brought two 30-litre barrels and just occasionally the beer was finished about five minutes before the end of exhibition.



PCO Martin Haloun at the Congress booth at ECM32.

During discussions at these meetings and subsequently, we have come to an agreement with some sponsors and exhibitors. We can announce that the platinum sponsor will be Rigaku, the combined gold-silver sponsor Bruker/Incoatec and the gold sponsor Anton Paar. ICDD is considering the bronze sponsorship. We hope to have even more companies interested in these [packages](#).



View from the Prague Congress Centre.

We are also discussing the social programme. The conference dinner will take place in the historic [National House of Vinohrady](#), not too far from the congress centre. The last day of the conference, 30 August, is a trip day. One of the trips we are going to offer is an excursion by train to the historical town of Český Krumlov in South Bohemia.

The registration system has been opened and accounts can be created [here](#). The system will be used to keep users informed of all important updates and for abstract submission, registrations (congress, workshops, events, trips) and payments.

IUCR ACTIVITIES

International Tables Volume H: Powder diffraction now available



We are pleased to announce the publication in print and online of the much-anticipated *International Tables for Crystallography Volume H: Powder diffraction*. This substantial volume, edited by C. J. Gilmore, J. A. Kaduk and H. Schenk, is the result of a huge amount of effort from the powder diffraction community, and we would like to thank the Editors and the authors for their outstanding dedication and hard work.

Powder diffraction is the most widely used crystallographic method with applications spanning all aspects of structural science. This new volume of *International Tables* covers all aspects of the technique with over 50 chapters written by experts in the field. The 932-page volume contains seven parts:

- Part 1 provides an introduction to the principles of powder diffraction.
- Part 2 covers instrumentation for laboratory X-ray studies, synchrotron, neutron and electron diffraction, 2D diffraction and special environments (temperature, pressure, magnetic fields, reaction cells). Sample preparation is also covered.
- Part 3 describes the different methodologies used in powder diffraction.
- Part 4 covers structure determination and validation.
- Part 5 discusses defects, texture and microstructure: stress and strain, grain size and thin films.
- Part 6 provides a useful review of available software.
- Part 7 describes applications to many areas of industrial and academic importance including macromolecules, zeolites, mining, ceramics, cement, forensic science, archaeology and pharmaceuticals. Both the theory and applications are discussed.

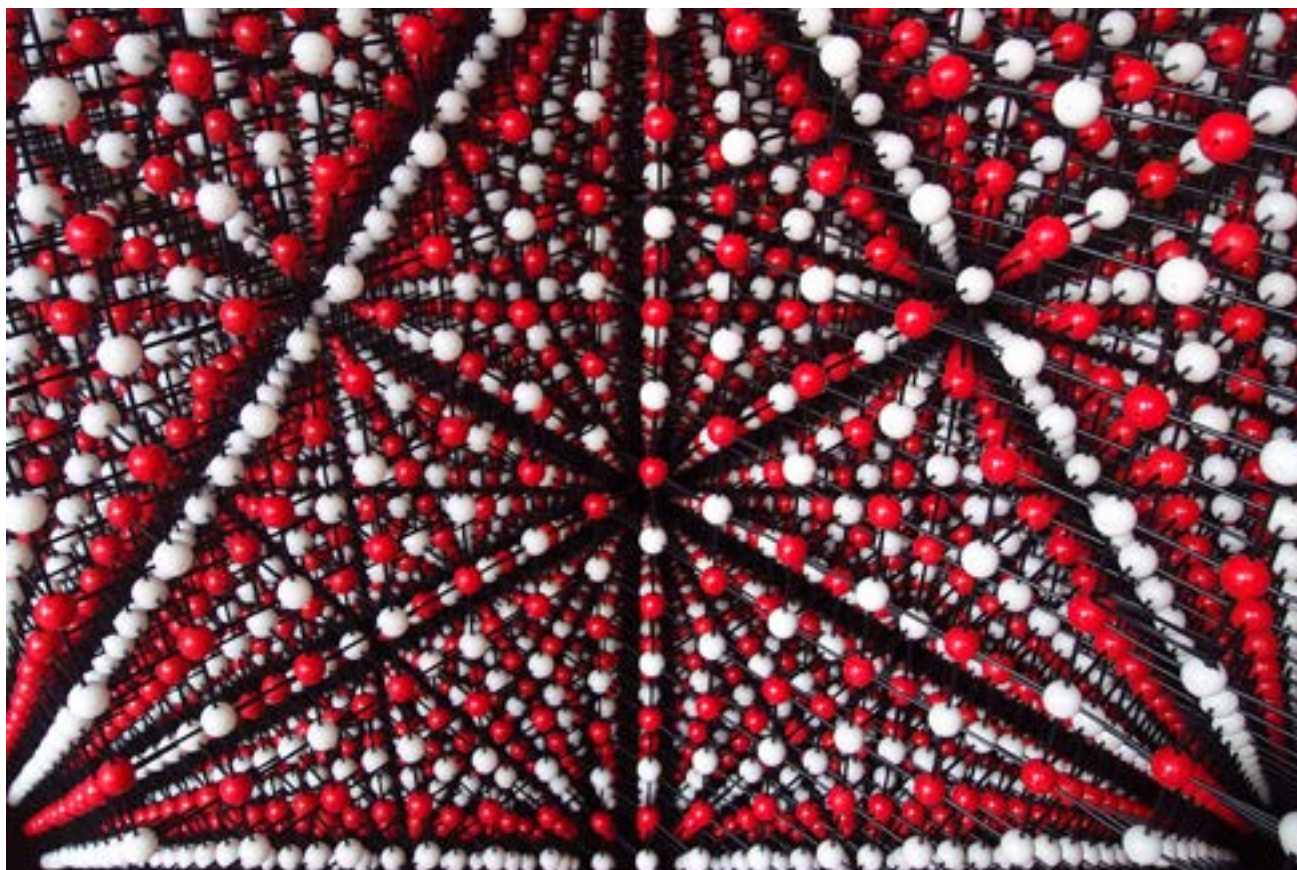
Volume H is the key reference for all powder diffractionists from beginners to advanced practitioners, and has been designed to be a practical volume without sacrificing rigour. Many examples of the method are discussed in detail and in several cases the data used are available to download.

Readers at institutions whose libraries have purchased perpetual access to the full set of *International Tables* will already have access to the online edition of Volume H. All the volumes are also available in print, with a 50% discount for [IUCr Associates](#) buying copies for personal use. For more information, please see [here](#).

OUTREACH

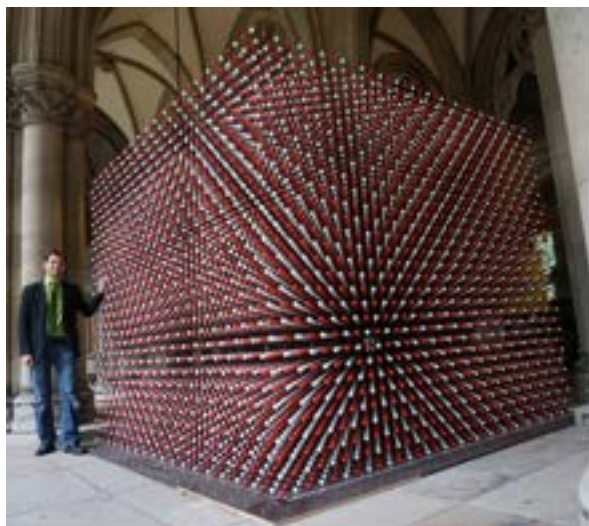
The largest crystal structure model in the world - an instructive tribute to milestones in the history of crystallography

Robert Krickl



View of the NaCl model down a threefold axis.

Participants in the recent European Crystallographic Meeting (ECM) at the University of Vienna, Austria, had the opportunity to witness a very special exhibit: an over 3-m tall model visualizing the periodic arrangement of atoms in crystals of the NaCl structure type, built from 40,110 red and white balls and, when put side by side, almost 11 km of connecting sticks, glued together with almost 500 tubes of glue. This is the largest ever physically modelled section of the arrangement of atoms in a crystalline solid. Previously a smaller precursor was confirmed by *Guinness World Records* as an official world record. Looking at the markedly bruised limbs of the tired person standing next to it giving information on how he built the model in several years of work, one may rightly ask: "Why on earth ...?". Well, there are several reasons.



The first model exhibited in Vienna in 2015 (left) and the even larger model exhibited at ECM32 in Vienna in 2019, with Robert standing beside both.

The first one is to do with an educational nature. I am an academic crystallographer who has dedicated his life to research and especially to science communication. The model was built to explain the concept of a crystal and to visualize the atomic arrangement of atoms in such a solid – not only a unit cell, but also one multiplied by translational symmetry! – to the general public. Indeed, this was very successful: from assembling in a public space and speaking to many school classes, kindergarten groups and members of the public from over 70 countries who visited the model to giving lectures on crystals and science history. Furthermore, parts of the model (which can be disassembled to modules to fit any required space) were shown at different educational events, museums, exhibitions and conferences. Some of you may remember the "small" part that was shipped to India to serve as an exhibition highlight at the 24th Congress and General Assembly of the IUCr in Hyderabad. Owing to its periodicity, the model provided not only amazing optical effects that served as very popular photo motifs but also a teaching tool for finding symmetry elements and crystallographic planes.



Robert Krickl with an official certificate for the World Record.

The second reason for building the model was to pay tribute to some great achievements in the past. The bulk of the model shown at the ECM in Vienna was finished in 2015 (consisting of 38,880 balls, which was officially registered as a world record back then). That year saw many anniversaries of important milestones in science history, especially connected to crystallography. Nearly 150 years ago, Wilhelm Conrad Röntgen began his academic studies that culminated in his discovery of X-rays, which happened exactly 120 years ago. Over 100 years ago, Max von Laue was awarded the 1914 Nobel Prize in Physics for discovering the diffraction of X-rays by crystals – proving that the latter exhibit a periodic arrangement of atoms. This is exactly what is visualized in the model. Also, following Laue's work, the father and son team William Henry Bragg and William Lawrence Bragg were awarded the Nobel Prize in Physics for 1915 for the first crystal structure determinations *via* X-ray diffraction. This had a major impact on science and our understanding of the world. One of the very first structures solved was the one of NaCl – the one shown in the model.



View of the model and W. H. and W. L. Bragg.

The model served as a place to celebrate the above anniversaries of science history. I was moved to tears on receiving a message from the descendants of W. H. and W. L. Bragg, who had heard about it via BBC coverage of the model. The following sentences are taken from a letter they sent, to be read out loud to the public and scientific community at the official record-setting festivity:

"Congratulations on your great achievement. My sister and I, the two daughters of William Lawrence Bragg, have been thrilled by your tribute to our father. He himself would have loved the whole idea. He was such a visual person. You could not have found a more original and satisfying way to celebrate his scientific legacy. [...]"

They also took a unique chance offered in the course of the project: everyone can immortalize themselves or their loved ones by sponsoring balls, which will henceforth be dedicated to that person with any individualized wording (these have even already been used as very special presents for weddings, birthdays and other occasions). There have been dedications to other famous crystallographers too. Companies can also participate. All are visible on the project's [homepage](#) and at the site where the model is displayed.

Further reverence was provided via philately. There was a special Austrian postage stamp issued on the world record model in 2015. It was given out at the site of the model on different special envelopes with special stamps, mostly on the occasion of the above anniversaries of science history. Apart from a first- and last-day cover, there was a special one on von Laue, Röntgen and father and son Bragg, as well as on the ECM (you can find all the information [here](#)).



First-day cover in honour of the Braggs.

So what happens next? The record has been achieved, but the project goes on. The model was built for educational purposes, *i.e.* to communicate science and visualize the nano-universe. It had to be removed from the University of Vienna but some modules are still being shown in different museums, schools and exhibitions. Everyone who wants to exhibit a part of or the entire model, is gladly welcome to [get in touch](#) ;).

In the end, the huge experience gained in the course of the construction was not wasted time. The balls were specially produced for this project in order to fit the stringent requirements of statics, durability and precision (bond angles and lengths have to be very, very accurate – otherwise you soon get a problem when stacking dozens of balls). Much investigation and testing took place to find a material and design with the best properties. I want to share this so one can experience the building of crystal structures oneself. I have developed special kits, which can be used at schools and universities, to easily build many different crystal structures – also huge ones. This fills an existing gap in teaching aids on inorganic chemistry, physics and crystallography. With the model and the new kits, I hope to contribute to the communication of science and the beauty of nature at all scales.

You can find more pictures and information on the model at the following:

<http://worldrecord.r-krickl.com> (English and German)

<https://www.facebook.com/worldrecordcrystalmodel/> (English)

<https://www.facebook.com/kricklrobert/> (German)

<https://twitter.com/KricklRobert> (English)

https://www.instagram.com/robert_krickl/ (German)

OUTREACH

Australian Women in Physics Lectureship 2019

Helen Maynard-Casely



Helen Maynard-Casely with the busts of W. H. and W. L. Bragg in Elder Park, Adelaide, Australia. [Photo taken by Andy Casely.]

Connecting researchers with school students is challenging. It is a challenge for the researcher to find time and funds to allow them to travel and speak to schools, and increasing demands on students' timetables means it is challenging to carve out time for extracurricular work. Add to this the challenge that your 25 million strong population is spread over an area the size of Europe then you can see the challenge that the Australian Institute of Physics (AIP) took on in getting new faces of physics into schools.

There's a real need for them to do this though. Nationally about 20% of those studying physics in Australia at university level identify as female. That's an improvement on numbers 20 years ago, but still something that sets physics in Australia apart from other STEM (Science, Technology, Engineering and Mathematics) subjects. Part of the modest rise may be down to the successful [Women in Physics lectureship](#) that the AIP has undertaken since 1997.

The motivation to start the lectureship started in South Australia where the local branch of the AIP wanted to honour the legacy of a colleague, Claire Corani, who had died in tragic circumstances. Conversations between other state branches led to the Claire Corani Memorial Lecture (as it is known in South Australia) being extended into a national lecture tour. The lectureship awardee undertakes a tour

of Australia, travelling to every state as well as Australian Capital Territory. It is awarded to someone who has (a) made a significant contribution in a field of physics research and (b) demonstrated public speaking ability.

This year it was me! It's rare now that crystallography is treated as its own subject and so most of us have to find homes in other departments, mostly it would seem in those of chemistry and biology. I found myself learning my trade of crystallography in a physics department, and have continued to use these skills in my research to discover the crystal structures of [materials formed all over the solar system](#). I'm now based at a central neutron scattering facility, the Australian Centre for Neutron Scattering, where I'm co-responsible for the high-intensity neutron diffractometer that we call Wombat.

I started with a bold title "How neutrons can save the world", and designed a talk that introduced the unique properties of the neutron and how we can use neutron scattering to study a range of problems, both on- and off-world. And before I knew it, it was time to set off. On the afternoon of 5 August 2019, I flew to Devonport in northern Tasmania to start the tour. Forty events later, I finished the tour at the Victorian "Girls in Physics" breakfast event held at Monash University. In that three and a half weeks, the tour had stretched from Hobart to Townsville, to Wollongong and Perth!



Helen speaking at St Patrick's College, Townsville. [Photo supplied by the school.]

A general highlight of the tour was that it really pushed my sphere of interactions with people! What I discovered on the tour is that recruiting and retaining specialist physics teachers here is a real challenge, both in regional (non-urban) and urban areas.

In terms of particular events, two stand out for me. The first was the visit to Oakey High School, in regional Queensland. It was organised by the school's physics teacher, Mitch Holgate, and Queensland AIP co-ordinator, Joanna Turner. Not only were the students there really engaged – definitely some of the best questions came from that session – but also the head of science, Jelena Edhouse, had baked a whole periodic table of cupcakes! A second event highlight was the visit to SIDES, the School for Isolated and Distance Education in Perth, organised by teacher and Western Australia AIP co-ordinator, Diana Tomazos. It was a totally different experience presenting to camera, with students tuning in from thousands of kilometres away. And they let me sign the studio door, a privilege usually reserved for famous people, like Nobel Prize winners!



Helen giving a public lecture at Monash University, Melbourne. [Picture taken by Matthew Lay.]

The tour took me to nearly every physics department in the country, and provided me with an unrivalled opportunity to get a great picture of the research that is undertaken in Australian physics. My skills in talking to a range of audiences have improved dramatically. A great feature of the tour is the range of events that are included – from talking on local radio, morning teas with physics students, and public lectures to seminars in physics departments around the country.

The AIP is currently looking for its next Women in Physics lecturer; for 2020 they are seeking an international-based researcher. If you have a lot to say about physics, identify as a woman and fancy a tour round Australia speaking to some very keen and interested students, [do apply!](#)

MEETING REPORT (IUCR SUPPORTED)

17th BCA/CCG Intensive Teaching School

Judith A. K. HowardHazel A. Sparkes



The 17th BCA/CCG (British Crystallographic Association/Chemical Crystallography Group) Intensive Teaching School in X-ray Structure Analysis was held at Trevelyan College, Durham, UK, from 6 to 14 April 2019. The school had an international feel with just over a third of the 80 students being based outside the UK, from a total of 15 different countries: UK, Argentina, Australia, Austria, Chile, Croatia, Finland, Germany, Ireland, Malaysia, Malta, Poland, Singapore, Spain and Switzerland. The atmosphere throughout the school was very friendly and supportive, which was noted positively in feedback from a number of the students and staff alike, with the variety of nationalities, different academic backgrounds and range of crystallographic experience creating an interesting environment both for learning and meeting new people.

The school has both a national and an international reputation for providing a good basis in crystallography that meant that we were once again heavily oversubscribed. The format of the biennial course has evolved as a result of feedback from students and staff and currently consists of a mixture of lectures and tutorials designed to help students improve their understanding of the lecture material. The course, as the name suggests, is intensive with a full timetable across the seven days providing the students with the opportunity to gain a good theoretical understanding of various aspects of crystallography from a single-crystal perspective. Following an introductory lecture shortly after arrival, the lecturers, Simon Parsons, Lukas Palatinus, Andrew Bond, Helena Shepherd, Richard Cooper and Mark Senn, guided the students through the following topics over the course of the week: Maths, Symmetry, Data Collection, Fourier/Patterson, Charge Flipping, Superspace, Direct Methods, Parameterisation, Least Squares, Refinement, Derivation of Results and Twinning. The tutorials are organised such that each of

the participants is assigned to a tutorial group for the week, which consists of eight tutees and a tutor who work together throughout the week to tackle a series of problems relating to the recent lecture material. This year we welcomed four new tutors: Christine Beavers, Laszlo Fabian, Claire Hobday and Hamish Yeung, as well as welcoming back Iain Oswald, Andrew Cairns, Nick Funnell, Amber Thompson, Claire Wilson and Hazel Sparkes. As usual the lectures and tutorials were held in the Sir James Knott Hall, which enables us to switch easily between formal lectures and tutorial work with minimal disruption. The accommodation and meals were provided in Collingwood College, which is less than a five-minute walk away but provided a pleasant chance for some fresh air and brief exercise during the day.

As is traditional at the school, apart from the Maths lecture on the first day, the evening activities are designed to be more relaxed and provide an opportunity for the students to mix with each other through a combination of educational and fun activities. On the Sunday evening, a successful bar quiz, organised by Professor Cooper, ended in a tight result with three of the teams being within one point of each other. The Monday evening session provided an introduction to Databases (Pete Wood) while the use of Synchrotron and Neutron facilities (Dr Beavers and Dr Senn) were highlighted on Tuesday. This year's student presentations, on the Friday evening, were organised by Dr Funnell and Dr Hobday. Each of the tutor groups put together a short (about five minutes) presentation on a crystallographic topic drawn from a hat earlier in the week in a style that was also chosen at random, e.g. *Local Structure in the style of Bake Off* or *The Bravais Lattice in the style of Bear Grylls* (two popular UK TV programmes). All of the groups put together creative and amusing presentations on their respective topics, which created an enjoyable evening with much hilarity. As with previous years the educational and entertainment value of each presentation was assessed by our elite panel of judges, the lecturers, who were very impressed by all of the entries.

The conference dinner on the Saturday evening provided the chance to thank all of the people who had contributed to the success of this year's school, the local staff, organisers, lecturers, tutors and students. The hard work and positive attitude from the staff and students alike all helped to create a very friendly school. After this year's school Professor Parsons stepped down as scientific director. We would like to thank him very much for his contribution over the last 10 years; his enthusiasm and drive have helped maintain the high standards of the course while keeping up to date with current developments. We are delighted that Simon is staying on the lecturing staff for the next school and very pleased that Professor Cooper has taken over as the scientific director and wish him every success.

Following on from the school, an optional hands-on *Olex2* workshop was held on the Sunday, run by Michael Bodensteiner and Oleg Dolomanov. This was well received by the ~40 registered participants who had the opportunity to use *Olex2* to apply structure solution and refinement concepts that they had learnt on the course to both test structures and their own data.

We would like to finish by saying thank you to all of the sponsors for this year's school: Diamond, IUCr, European Crystallographic Association, CCG, Industrial Group, Oxford Cryosystems, Bruker, Rigaku Oxford Diffraction, Cambrex and the National Crystallography Service. Without the financial support from these organisations we would not have been able to help as many students attend the school or run it so successfully and we are very grateful for their continued support.

IUCr support

The funds kindly provided by the IUCr were used to help three PhD students with contributions towards their subsistence; they share their experiences below.

Owen Missen (Monash University, Australia)



Despite its rarity, tellurium is a major component of over 170 minerals due to the variety of tellurium oxidation states available – and the corresponding variety of crystal structures tellurium can form. Single-crystal X-ray diffraction is a gold standard in mineralogy to (help) show that a mineral is unique. Thus, a thorough knowledge of crystallography is essential for my research. In order to broaden my crystallographic knowledge, I applied to attend the 17th Durham Crystallographic School. A bursary from the IUCr was extremely helpful in enabling me to attend the School. In addition to the obvious educational benefits of attending a week-long intensive School, I also met many other young crystallographers and also the professor who recommended the School to my supervisor.

My mineralogical research (two-year Masters, currently nearly a year into my PhD) focuses on the ~20 minerals containing tellurium and oxygen that do not have reported crystal structures, requiring thorough re-investigation. Prior to the School, I had published three unique tellurium mineral structures after re-investigating old and poorly characterised minerals, each requiring detailed analysis of the crystal chemistry. Attending the School broadened my understanding of the underlying mathematics and rationale underpinning crystallography. Lectures on topics including symmetry, structural refinements and twinning (to name a few) will all help me as I continue to research mineralogical crystallography into the future. I express my gratitude again to the IUCr and hope to disseminate my future crystallographic results at IUCr conferences in years to come.

Federico Movilla (University of Buenos Aires, Argentina)



Crystal engineering is the design and synthesis of crystalline solids with a particular purpose and specific properties. Three distinct activities can be identified as part of this definition, which themselves form a continuous sequence: (i) the study of intermolecular interactions, (ii) the study of packing modes in the context of these interactions with the aim of designing a strategy for crystal construction and (iii) the study of crystal properties. Thus, as a starting point, it is essential to perform high-quality single-crystal X-ray diffraction studies that lead successfully to the molecular and supramolecular structure of the

studied systems. In the Crystal Engineering and Structural Chemistry Group of the Inorganic Chemistry Department at my university, we develop different projects based on amino acid and peptide derivatives using crystal engineering and crystallography. Thus, the continued training of the members of the group, especially PhD students, in these fields is always encouraged. I joined this group as an undergraduate student, and am currently in my first year as a PhD student. Consequently, I applied to attend the 17th BCA/CCG Intensive Teaching School in X-ray Structural Analysis at Durham University, one of the best in the area. The bursary granted to me made my participation in the school possible as the money in our grants available for traveling is very scarce.

All of the topics covered by the school were very useful, and I followed lectures given by some of the main researchers and developers of modern crystallography, which were essential to improve my knowledge. Outside the classroom, being in contact with young scientists from all over the world and having the opportunity to listen and share diverse ways of solving everyday crystallography issues was a fruitful experience and also let me create a new working network.

Nazhirah Nasri (University of Putra Malaysia, Malaysia)



Metal-organic frameworks (MOFs) are a class of porous materials constructed from various organic linkers and metal ions. Among the reported MOFs, zeolitic imidazolate frameworks (ZIFs) have emerged as a promising subfamily of MOFs, possessing the advantages of both zeolites and MOFs. ZIFs are constructed from transition metals such as Zn^{2+} and Co^{2+} bridged to N-donor atoms of the imidazolate linkers in a tetrahedral cluster to form a neutral large framework. Zn^{2+} is surrounded by imidazolate linkers (Zn-Im-Zn), which is similar to the role of Si in zeolites, which is bonded to oxygen (Si-O-Si). Coincidentally, the bond angles of zeolites and ZIFs are similar. Nowadays, ZIFs have been investigated as drug carriers due to their special properties such as high surface area, large pore volume and high thermal and chemical stability.

In my PhD studies, I have been working on mixed-linker ZIFs and synthesised ZIFs using two, three and four different imidazolate linkers mixed with Zn^{2+} to produce large frameworks with a high surface area. The atomic position in the crystal structure and specific topology have allowed various coordination geometry due to the variation of imidazolate linkers in the crystal structures. However, these ZIFs are always associated with disorder due to solvent molecules and twinning problems.

The bursary from the IUCr allowed me to attend the 17th BCA/CCG Intensive Teaching School in X-ray Structure Analysis in Durham, and I learned a lot about the fundamental theory behind X-ray crystallography. The knowledge obtained throughout the course has helped me to solve single-crystal X-ray diffraction data, especially the disorder problems within ZIF structures. I also had the opportunity to meet great researchers in crystallography and obtain new ideas and perspectives for my research project. I also had a fun learning experience and made new friends.

MEETING REPORT (IUCR SUPPORTED)

RapiData 2019

Silvia RussiClyde SmithJeney Wierman



RapiData 2019 co-organizers and IUCr bursary awardees. From left: Jeney Wierman, Esdras Carrizosa Carbajal (Mexico), Silvia Russi, Aliny Bastos (Brazil), Angela Escudero Garcia (Mexico), Sunil Singh (Singapore) and Clyde Smith.

On 5–10 May 2019, RapiData@SLAC course co-organizers Clyde Smith, Silvia Russi and Jeney Wierman brought together over a dozen specialized experts from around the world for RapiData 2019, to share lectures and tutorials on the many aspects of an X-ray macromolecular crystallography experiment. Guest lecturers included Raji Edayathumangalam (Columbia), Andreas Foerster (Dectris), James Fraser (UCSF), Ana Gonzalez (MAX-IV), James Holton (UCSF), Brian Kobilka (Stanford), Dorothee Liebschner (LBNL), Jim Pflugrath, Harry Powell (DLS), Nick Sauter (LBNL), Bob Sweet (BNL), Andrea Thorn (Julius-Maximilians University Wuerzburg) and Clemens Vonrhein (Global Phasing).

The RapiData@SLAC students consisted of a diverse class of 42 national and international students, ranging from undergraduate and graduate students to postdoc scholars and research associates. One important mandate for all the previous RapiData courses has been to encourage attendance by young scientists from Latin America with the assistance of scholarships from the IUCr. As always, this IUCr support is critical, as the amount of funding available to research institutions in Latin America, Africa and South East Asia for student travel grants has severely diminished over the years. Moreover, as with last year, we have had to substantially increase the size of the awards in order to facilitate attendance of participants from this region. We awarded four scholarships to pay for accommodation and/or travel and subsistence expenses to attend RapiData 2019. The recipients were selected based on a letter of recommendation by their supervisor stating how the student would benefit from attending the course

and how their attendance will allow for the dissemination of the practices taught at the course in their home laboratories. The awards were presented during a ceremony on the last day of the course. The co-organizers are also very grateful for the support Stanford Bio-X, MiTeGen and Dectris provided for the program.

At the start of the workshop students attended lectures about macromolecular crystallography and the complementary structural biology techniques of cryoEM and BioSAXS, as presented by Wah Chiu (Stanford) and Thomas Weiss (SSRL-SMB), respectively. The second half of the workshop was split into nine separate tutorials taught in small groups that focused on hands-on data collection at the beamlines and data processing and data analysis with experts in small classroom settings. Additional instructors for the hands-on tutorials included from the Phenix group (Li Wei Hung, Billy Poon, Nigel Moriarty), CCP4 (Andrey Lebedev), Global Phasing (Claus Flensburg) and HKL (Ivan Shabalin), and from SSRL and Stanford University (Aina Cohen, Tzanko Doukov, Edgar Estebanez, Daniel Fernandez, Artem Lyubimov, Irimpan Mathews, Tsutomu Matsui, Ivan Rajkovic, Silvia Russi, Clyde Smith and Jeney Wierman). Students were invited to bring their own crystals to learn the tips and tricks of data collection specific to their own research. Students were given access to the novel data collection capabilities at SSRL, such as controlled humidity data collection and complementary UV-visible absorption microspectrophotometry. Here, the tutors could focus on individuals and answer more personalized questions, such as, “how do I process my challenging dataset?” Although the lecture and tutorial schedule was jam-packed from sun-up to sun-down, it was only natural to include much-needed breaks to give students and experts time to casually mingle and continue mentoring over meals and coffee.

Beyond having crystallography experts gathered in one place, an added benefit of being hosted at SLAC was direct access to experimental facilities at both SSRL and at the Linear Coherent Light Source-II (currently under construction). Students toured the SMB beamlines and both the Coherent X-ray Imaging (CXI) and the Macromolecular Femtosecond X-ray Crystallography (MFX) instruments at LCLS-II [thanks to tour guides Aina Cohen and Meng Liang (LCLS-CXI)]. The co-organizers added a new feature to the program this year in the form of two prominent guest lecturers on separate days. These two experimentalists, who have collected data at SLAC’s LCLS and SSRL, gave pre-dinner lectures drawing direct connection between the experimental techniques being taught in the course and the impact of their results. The guests were then invited to dine with the students and tutors at a catered dinner. The first guest lecturer, Brian Kobilka of Stanford University, rounded out the first day of tutorials with a captivating presentation on structural approaches to understanding G protein-coupled receptor (GPCR) signaling. Armed with humorous quips about the ups and downs of data collection, Professor Kobilka related his past GPCR experiments and framed the place of GPCR signaling, not only in history, but also in biology – a look into the work that awarded him a Nobel Prize in Chemistry in 2012. As approximately half of all medications used today make use of GPCRs, his lectures underlined the importance of the X-ray data collection toolbox the students were learning and mastering through the RapiData@SLAC course. As a wonderful conclusion to rapid-fire five day lecture and tutorial circuit, James Fraser of University of California San Francisco presented an intriguingly titled talk, “Conformational Change We Can Believe In!”. His animated presentation described the influence of conformational change within protein structures at varying temperatures and highlighted the recently renewed interest in room-temperature data collection. Here was a direct tie to the newly added room-temperature data collection lectures and tutorials within the RapiData@SLAC circuit.

As in previous years, the organizers presented the IUCr and Stanford Bio-X travel scholarships to students on the final day. The organizers, instructors, tutors and students all shared their satisfaction and enthusiasm for the course, and look forward to continued RapiData courses. With that in mind, planning is underway for the 2020 edition of RapiData@SLAC to be held from 30 March to 4 April.

MEETING REPORT (IUCR SUPPORTED)

Seventh International School on Biological Crystallization

Juan Manuel García-Ruiz



The Laboratory of Crystallographic Studies (CSIC-UGR) successfully organised the Seventh [International School on Biological Crystallization](#) (ISBC2019) on 26–31 May 2019 in Granada, Spain, under the auspices of the IUCr through its Commissions on Crystal Growth and Characterization of Materials, Biological Macromolecules and Crystallographic Teaching, with the support of the International Doctoral Summer School Programme of the School of Science, Technology and Engineering of the University of Granada, the Spanish Royal Society of Chemistry and the Spanish Specialized Group of Crystallography and Crystal Growth.

As in previous years, the event took place downtown in the beautiful city of Granada. The school attracted the interest of postgraduate/postdoctoral students as well as research scientists from industry and academia who routinely deal with crystallization processes but seek fundamental knowledge on the crystallization phenomena and the behaviour of crystallizing solutions. The students came to Granada to learn from top quality international speakers, hear case study presentations, watch practical hands-on demonstrations and present their research in poster sessions.

During the five-day school, several subjects related to the field of the crystallization of biological macromolecules were covered including hot topics such as crystallization of large crystals for neutron diffraction, tiny crystals for XFEL studies and the crystallization of membrane proteins and large macromolecular complexes. As in previous years, the demonstrations fair was very successful with much

positive feedback from many participants. The two round-table discussions were also highly appreciated among tutors, academics, students and industrial representatives.

Attendance

The turnout of the school was excellent having a total of 96 participants from 20 different countries, most of which were students (51), speakers (28) and academics (10), the rest being industrial representatives and exhibitors. The participants were supported by a team of 15 people from the organization.

A considerable effort was made to provide financial support to as many students as possible. All 30 applicants were awarded a bursary to attend the school, including all of the students travelling from outside Spain.

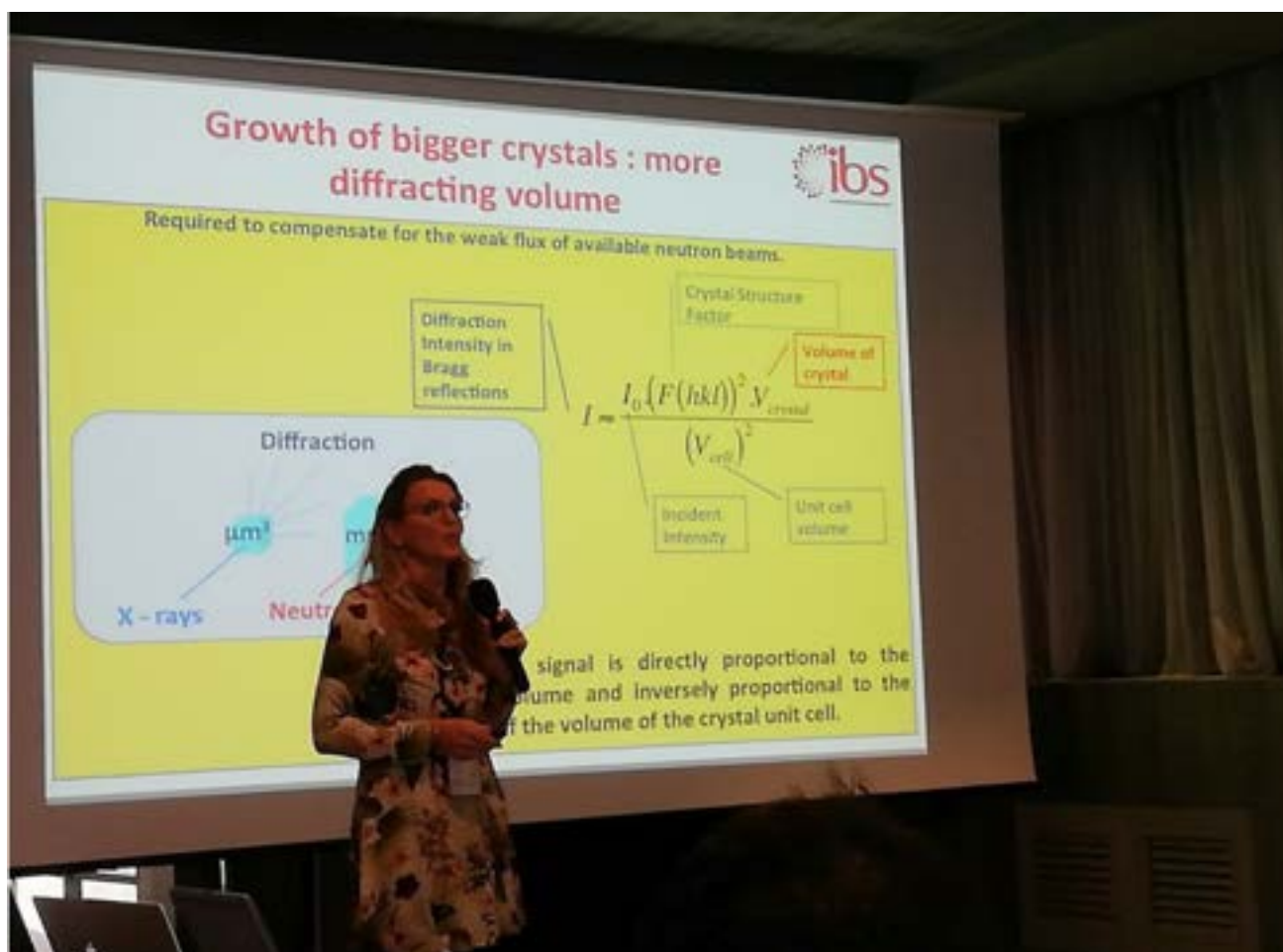
Programme

Monday started with an introduction to the school and was fully dedicated to explaining the whole process of crystallization “From solution to protein crystals”, from the purification and preparation of protein solutions to the basic concepts of crystallization, nucleation, phase diagrams, crystal growth kinetics and different crystallization techniques.



Terese Bergfors explaining how to interpret crystallization results.

Tuesday was devoted to special hot topics including femtosecond crystallography, microseeding, microfluidics, how to grow crystals for neutron diffraction, and the crystallization of membrane proteins and large macromolecular complexes. On Wednesday there were sessions on especially relevant topics such as optimization of crystal growth for neutron diffraction, SAXS, EM etc.



Monica Budayova explaining how to optimize crystal growth for neutron macromolecular crystallography.

Thursday was dedicated to the very popular demonstrations fair, at which specialists offered 21 short (20–40 minute) practical sessions at scheduled times. Participants were free to choose which sessions to attend so that they selected their own learning programme *a la carte*. The demonstrations fair proved to be an excellent teaching tool as it provided students with plenty of opportunities to interact on a personal basis with the teachers and to watch closely how to perform crystallization experiments. The last day of the school had two round-table discussions, the first on convergent techniques, including diffraction, XFEL, micro-ED, SAS, NMR, cryo-EM and the future of protein crystallization, the second on publishing results.



Ivana Kuta Smatanova (second from right) and Pavlína Řezáčová (right) showing the students how to perform vapour-diffusion (hanging and sitting drops) experiments.

There were poster sessions on Monday, Tuesday and Wednesday, which proved to be very valuable, allowing discussion of scientific work. The poster winners (see Table 1), selected by an international panel of lecturers composed of Bernhard Rupp, Abel Moreno and Claude Sauter, gave a 5-minute presentation on Friday morning.

Table 1. Poster prize winners in ISBC2019.

Student	Affiliation	Prize
Rosanna Caliandro	Free University of Bolzano-Bozen	IUCr
Ines Trindade	Instituto de Tecnologia Química e Biológica António Xavier	IUCr
Rebecca Jernigan	Arizona State University	IUCr
Dorota Kubacka	University of Warsaw	Crystals-LEC
Diana O Silva	iBET- Instituto de Biologia Experimental e Tecnológica	PDBe
Mari Carmen Salinas Garcia	University of Almeria	Garland



One of the lively poster sessions during ISBC2019.

Social events

In addition to the scientific course, there was a parallel social programme, which consisted of welcome cocktails on Sunday, a night tour of the Moorish gardens of the Alhambra on Tuesday and Wednesday, and a Flamenco dinner party on Thursday in the traditional district of Albayzin, which is renowned worldwide for its flamenco music.



The Flamenco party on the Thursday evening.

Final notes

All in all, ISBC2019 was an enriching experience for all of those involved, triggering many fruitful scientific discussions. The positive approach, openness and active participation of each participant made it a wonderful experience that would be worthwhile to repeat in the future.

Finally, we would like to express our gratitude to all participants: the teachers for their full commitment and the students and colleagues from academic and industrial backgrounds for believing in these crystallization schools. We also wish to express our heartfelt thanks to the committee for their essential contribution to the success of the school. Last but not least, we would also like to express our gratitude to the sponsors and exhibitors for their great support.

MEETING REPORT (IUCR SUPPORTED)

Fourth Summer School on Mathematical Crystallography

Massimo Nespolo



The IUCr Commission on Mathematical and Theoretical Crystallography ([MaThCryst](#)) has organized the fourth [Summer School on Mathematical Crystallography](#) in Nancy, France (the first edition was organized in 2005, the second and third in 2010). The school was held at the [Faculty of Sciences and Technologies](#) of the [Université de Lorraine](#) on 3–7 June 2019 and received financial support from the [IUCr](#), the [European Crystallographic Association](#), the [French Crystallography Association](#), the [French Society of Mineralogy and Crystallography](#), the [Grand Nancy Metropolitan Government](#), the [Doctoral School of Physics, Chemistry and Materials](#) and the [CRM²](#) laboratory.

The school aimed at providing a solid background in fundamental crystallography, with special emphasis on those aspects that are taught less and less in university curricula. The first two days were entirely devoted to the fundamentals: symmetry, periodicity, lattices, point and space groups in two and three dimensions, and stereographic projection of crystal forms and orthogonal projections of space groups and equivalent atomic positions. The third and fourth days concentrated on matrix algebra applied to the description of crystal structures, crystallographic calculations, change of coordinate systems and their effect on the Hermann–Mauguin symbols of space groups, normalizers of point and space groups, equivalent descriptions of crystal structures, and group-subgroup relations of point and space groups. The theory was accompanied by exercises on the [Bilbao Crystallographic Server](#). The last day was dedicated to reciprocal space: introduction to the reciprocal lattice, geometric interpretation and derivation of reflection conditions, symmetry considerations and restraints and constraints in structure

refinement from single-crystal X-ray diffraction data. The lecturers were [Massimo Nespolo](#) (Université de Lorraine), [Gemma de la Flor Martin](#) (Karlsruhe Institute of Technology, Germany) and [Benoît Guillot](#) (Université de Lorraine), who were assisted by two tutors, [Berthold Stöger](#) (Technical University of Vienna, Austria) and [Isabella Pignatelli](#) (Université de Lorraine).

The school was attended by 40 participants representative of 20 nationalities, and of 26 institutions from 13 countries. Ten grants to students and young scientists (half of which were female) were attributed to facilitate their participation. A photo gallery is available [here](#). Slides and didactic material are available from the school website and from the [MaThCryst repository](#).

Forthcoming activities of the commission are announced on the [MaThCryst Meetings and Schools page](#).

MEETING REPORT (IUCR SUPPORTED)

53rd Course of the International School of Crystallography: Magnetic Crystallography

Annalisa Guerri



The attendees enjoyed a team game to celebrate the International Year of the Periodic Table.

The 53rd Course of the International School of Crystallography (ISCoC) on the subject of magnetic crystallography was held in Erice (TP), Italy, on 31 May–9 June 2019 and was organized by the IUCr Commission on Magnetic Structures. The scientific directors were Branton Campbell (Brigham Young University, USA), Maria Teresa Fernandez-Diaz (Institute Laue-Langevin, France) and Manuel Perez-Mato (Universidad del Pais Vasco, Spain). There were 57 selected participants coming from 17 different countries.

The school included a roughly 50/50 combination of lectures and hands-on workshops. Three hours of workshops were held each morning with two sessions conducted in parallel. The state-of-the-art computational tools presented in the workshops included *FullProf*, *JANA2006*, *SARAH*, the Bilbao Crystallography Server, the *ISOTROPY* Software Suite, *GSAS-II* and *TOPAS*. Both introductory and advanced tutorial exercises were provided. Topics included the experimental determination and communication of magnetic structures, the theoretical and mathematical foundations of magnetic symmetry and representational analysis, and a wide variety of applications. More than 40 abstracts were submitted and 10 were selected for oral presentations.

The two poster sessions held to showcase participant research were also of very high quality and well attended during the school. Three of these posters were selected by a panel of judges for awards. The

technical program ended with a one-hour panel discussion of questions submitted by the participants. The rich social program, which also included the celebration of the International Year of the Periodic Table through a team game, created a very relaxed atmosphere thanks to which participants and organizers became personally acquainted and fostered new long-term friendships and collaborations.



MEETING REPORT (IUCR SUPPORTED)

14th International Symposium on Macrocyclic and Supramolecular Chemistry

Pierangelo Metrangolo Francesca Baldelli Bombelli Giancarlo Terraneo



IUCr Poster Prize winners Larissa von Krbek and Roy Lavendomme (third and fourth from left) flanked by conference chairs Francesca Baldelli Bombelli, Pierangelo Metrangolo and Giancarlo Terraneo.

The [14th International Symposium on Macrocyclic and Supramolecular Chemistry](#) (ISMSC2019) was held in Lecce, Italy, on 2–6 June, 2019, and chaired by Pierangelo Metrangolo, Francesca Baldelli Bombelli and Giancarlo Terraneo (Politecnico di Milano, Italy).

Background

The ISMSC originated from the merging of two long-running and independent but closely related symposia, the International Symposium on Macrocyclic Chemistry (ISMC – established in 1977) and the International Symposium on Supramolecular Chemistry (ISSC – established in 1980). Over the years, the two fields have dramatically expanded while also becoming closely aligned. After the first ISMSC, which was held in Victoria, Canada, in 2006, the symposium was set as an annual conference and in the five past years was held in Quebec City, Canada (2018); Cambridge, UK (2017); Seoul, South Korea (2016); Strasbourg, France (2015); and Shanghai, China (2014).

The objectives of ISMSC2019 were to

- provide a forum to discuss all aspects of macrocyclic and supramolecular chemistry, and also topics on materials and nanoscience, following the spirit and style of the preceding conferences

- offer networking opportunities among peers, recognized leaders in the field, young scientists and students
- develop new aspects of macrocyclic and supramolecular chemistry
- push the boundaries of macrocyclic and supramolecular chemistry and related interdisciplinary fields across the full spectrum of science and technology
- expose the broad macrocyclic and supramolecular community to the work and accomplishments of promising young investigators and thereby promote their career development.

Participation

The ISMSC2019 brought together 712 active participants from 43 countries, representing both academia and the private sector. The scientific program included 2 lectures from the 2016 Nobel Laureates in Chemistry (Sir James Fraser Stoddart and Bernard L. Feringa) as well as 4 award lectures including the 2019 Izatt-Christensen Award (Luisa De Cola), Cram-Lehn-Pedersen Prize (Xiaopeng Li) and Sessler Early Career Researcher Prize (Ross Stewart Forgan) winners. ISMSC2019 also hosted the Natural Product Reports Emerging Investigator Lectureship (Konrad K. Tiefenbacher). A total of 22 keynote, 24 invited and 12 oral lectures, as well as 24 short paper lectures and 2 poster sessions were scheduled, where 550 posters were displayed.

Outcomes and results

The ISMSC2019 hosted renowned researchers who work in a wide range of different fields such as organic electronics, nanotechnology, biology, medicine and materials science to discuss their cutting-edge research results, in which supramolecular chemistry (the use of intermolecular interactions to build up self-assembled systems) is the tool for developing innovative materials, devices, macromolecules, nanovectors *etc.*

This symposium promoted the establishment of new interdisciplinary areas of research between chemistry, in particular supramolecular chemistry and nanomedicine, bioengineering and organic electronics. The scientific advancements discussed during the conference were shared with the international chemistry community.

ISMSC2019, beyond providing a platform for scientists from different disciplines to brainstorming and promoting cross-disciplinary collaborations, represented a great opportunity for junior researchers and PhD students to present their work and discuss new ideas with well-established leaders in their field of research.

During ISMSC2019, a public lecture was delivered by Sir James Fraser Stoddart to present the world of supramolecular chemistry and the long scientific journey that has brought him to receive the Nobel Prize in Chemistry 2016. More than 800 high school students as well as citizens attended this lecture.

Furthermore, ISMSC2019 was spread over several historical venues in the city of Lecce, such as the city theater, Teatro Apollo (opening ceremony); Monastero degli Olivetani (lunches and poster sessions); Torre del Parco (speakers' dinner) and Chiostro dei Domenicani (banquet), which gave a unique opportunity for attendees to experience the architectural and historical beauties of this southern part of Italy.

ISMSC2019 provided 52 Young Researcher Grants, including 5 IUCr Young Scientist Awards. Giulia Regeni (TU Dortmund, Germany), Paolo Mazzeo (Università degli studi di Parma, Italy), Shiqiang Wang (University of Limerick, Ireland), Vignesh Athiyarath (Indian Institute of Science Education and Research, Thiruvananthapuram, India) and Asia Marie S. Riel (University of Montana, USA) each received a contribution towards their travel and/or accommodation expenses.



Giulia Regeni



Paolo Mazzeo



Shiqiang Wang



Vignesh Athiyarath



Asia Marie S. Riel

In addition, 30 poster prizes were awarded during the banquet. The IUCr prizes were awarded to Larissa K. S. von Krbek (University of Cambridge, UK) for her poster "Allosteric regulation of anion exchange in an Fe_4L_6 tetrahedron" and to Roy Lavendomme (University of Cambridge, UK) for "Self-assembly of palladium(II)-templated covalent macrocycles, cages and larger structures".

MEETING REPORT (IUCR SUPPORTED)

Ninth Zürich School of Crystallography

Hans-Beat BürgiTony Linden



The Ninth Zürich School of Crystallography: Bring Your Own Crystals returned from Tianjin, China, where the eighth school took place, to the Department of Chemistry at the University of Zürich, Switzerland, from 16 to 27 June 2019. The 20 participants (12 female) comprised 1 BSc, 1 MSc and 15 PhD students, 1 postdoc and 2 junior academics. They came from 13 countries: Brazil, Croatia, Finland, Germany, Greece, Hong Kong, India, Morocco, Portugal, Russia, Slovenia, Switzerland and Tunisia.

The central goal of the school is to equip each participant with enough knowledge of the theory and practice of X-ray diffraction and single-crystal small-molecule structure determination so that they can competently determine their own structures when they return to their home laboratory. The daily schedule is a blend of lectures, exercises and practical work.

In our experience, symmetry is a notoriously difficult topic. In addition to lectures, we use tutorials with small groups of five students and one or two tutors, which has proven to be effective.



Left: Lukáš Palatinus lecturing on difference Fourier syntheses. Right: Tony Linden leads a tutorial on point groups.



Students with Céline Besnard (left) and Pascal Schouwink (right).

On the third day, the students worked with the crystals they had brought to the school; they selected a crystal, put it on one of the five diffractometers accessible at ETHZ and UZH, and measured and processed a dataset. The diffractometers included the modern Bruker Venture D8 and Rigaku Oxford Diffraction Synergy instruments, which are impressive in terms of speed, the availability of two radiation wavelengths and detector sensitivity.

In preparation for interpreting their own data, the students solved three example structures of varying degrees of difficulty that were designed to allow the participants to see behind the button pushing, to learn about the actual procedures going on when various operations are performed and to interpret whether or not appropriate results are obtained. Each participant then works on the dataset collected from their own sample.

In our fully equipped computer classroom, we used the *Olex2* software once again this year and found it to be quite suitable in the school environment. The ease of use of *Olex2* allows us to demonstrate more aspects of structure solution and refinement in a shorter time. The ever-expanding range of special tools and options in the program for easy handling of special modelling issues, such as disorder, is very useful. As usual, we had our very popular 2:1 student:tutor ratio.

Each day concluded with a short discussion where participants could express their feelings about their experience that day. All of the participants were very enthusiastic and their eagerness and dedication were maintained throughout the school. Some were just getting their feet wet in the field of crystallography, whereas others were more experienced, but all participants came away having learned something new and feeling better equipped to tackle structure determination on their own. Everyone mixed well, chatted eagerly together and became friends. When the youngest participant, Liza, had her birthday midway through the school, her companion students got her cakes and candles and sang...

On the final day, each participant sat a two-hour written exam either to obtain ECTS credit points or to self-test their knowledge.

At the end of each afternoon, after the classes and feedback session were over, the day was not yet finished. Students and tutors ate dinner together and got to know each other on a more personal level. It is not unusual for the tutors to be asked to clarify undigested course material after the meal and sometimes deep into the night.

Before returning home, all participants met for a Chinese banquet. Each participant received a certificate and a copy of *Crystal Structure Refinement, a Crystallographer's Guide to SHELXL* by Peter Müller, kindly donated by the IUCr and OUP.

The questionnaire filled in by the participants provided overwhelmingly positive feedback. The perennial criticism is the intensity of the school. Participants often wish for more breaks so they can digest the content better. To do so would add accommodation costs and require more time commitment from our team of dedicated tutors, so we feel people have to accept that it is an intense block course, unlike a semester course. The personal impressions of two participants are given below.

We gratefully acknowledge the generosity of the sponsors and supporters: Department of Chemistry of the University of Zürich; Swiss Society of Crystallography; Cambridge Crystallographic Data Centre; European Crystallographic Association; IUCr; Oxford University Press; Rigaku Oxford Diffraction; Dectris Ltd; Oxford Cryosystems; Bruker AXS; Hotel Coronado, Zürich; the Chemistry Platform of the Swiss Academy of Sciences and Michael Woerle for taking many photographs, some of which are in this report.

Guratinder Kaur (Paul Scherrer Institute, Switzerland)



Guratinder Kaur (left) receives her certificate and book from Tony Linden (centre) and Hans-Beat Bürgi.

It is an honour and pleasure to pen down my experience during "The Zürich School of Crystallography 2019", which has excelled in terms of the quality of teaching, tutorial sessions, layout of the course and the venue. When I started my PhD in October 2016, I heard about this school but the deadline had already passed so unfortunately, I could not apply for it. I felt terribly sad and since then I had been waiting for the next announcement. The wait came to an end in 2019 and has been worthwhile.

Initially I was bit concerned about the duration and the efficiency of the school as usually such long-term schools or workshops fail to stay consistent throughout the mentioned time span. This school has exceeded all my expectations as it was such an incredible platform for beginners in crystallography. I was amazed with the versatility of the course module including international participants with entirely different academic backgrounds. My other major concern was how intense the course was going to be; however, small tea/coffee breaks during the day and a carefully planned schedule made everything absolutely effortless. There must be a delicate balance that has to be maintained to keep the participants interested and motivated until the end. After attending the school, my experience is that organizers have spent significant time working out the best way to arrange everything, and this made a huge success of ZSC19. The atmosphere of the university and the two students per one tutor ratio were incredible. The accommodation in the hotel is just perfect as it is so convenient and relaxing to commute.

I had never taken a course in crystallography before, but after attending this school, I feel that I would not have had more success at any other school. Having started my PhD in diffraction, I really had a hard time understanding my research problems. In fact, I lacked the vision to appreciate the beauty of symmetry and crystallography. These are somewhat difficult concepts and were thoroughly explained in several ways to us by the tutors at ZSC19 who were so passionate about teaching and sharing their experiences with the participants and very eager to answer questions at any time, participating in never-ending scientific discussions with the students – even until late in the evening!

As crystallography is a fundamental concept used in almost every scientific field, I was skeptical about the several different topics that may have little relevance to my work. However, this was not the case and I learnt a lot from all the talks. The invaluable practical sessions were excellent, especially being able to analyze the data from our own crystals as well as data that were also obtained on the instruments in our home institutions. Interacting with tutors and other participants and socializing with them was great. It was so motivating and rewarding that, at the end of a day, one can actually give his/her sincere opinions about the lectures and practical sessions as feedback.

From this course I feel that I have enhanced and refined my knowledge of crystallography and also how to implement this tool to tackle difficult research problems. This knowledge is crucial for my current position as well as in my future career, and hopefully I will be able to use and pass on this information further in the near future. The course has exposed me to one of the most beautiful disciplines and given me an appreciation for crystallography. I lacked confidence in this area before coming here. I highly recommend this course to anyone who wants to see the world of crystallography under the guidance of its pioneers. Once again, I must say, hats off to the commendable job done by the organizers. Thank you!

Helena Brodnik Žugelj (University of Ljubljana, Slovenia)

Hans-Beat Bürgi (right) hands a certificate and book to Helena Brodnik Žugelj.

As an organic chemist I am always faced with the uncertainty of synthesizing the correct product. And even though there are several methods to help determine what compound you have prepared, I believe that having an X-ray structure of that compound indubitably confirms what you hold in your hand.

For those who wish to learn the theoretical background and gain practical experience of X-ray diffraction from the very beginning (how to grow your crystals) to the final touches at refining and publishing your structure, then the Zürich School of Crystallography is the best way to do it. Looking back at my experience I can honestly say I would do it again. Even though it is an intense 10-day course covering both theory and experimental work, the amount of knowledge and level of expertise presented gives you valuable experience you will never forget. It is a highly interactive school, as you get the chance to work on a diffractometer, as well as gain as much theory needed to later solve your own crystal structures. An important value the school offers is being able to work, study and debate with ten highly experienced crystallographers, who become your tutors for the whole time in Zürich. Each tutor is assigned only two participants, which makes this school a luxurious opportunity to obtain valuable knowledge. During the school the tutors are always available and willing to help you understand certain topics you find yourself struggling with. From my point of view, the friendliness and level of expertise of all the tutors truly places this school at the very top.

The motto of the Zürich School of Crystallography is “bring your own crystals”, which means you are given the opportunity to send your crystals prior to your visit, so you can work on your structure once you are there. This is especially valuable for those who struggle with solving more difficult structures. Hence, having so many experts at hand can really help you understand and solve your structure.

The school was very well organized as all the lectures and exercises were carried out smoothly. Everything is prepared before you even arrive from lecture notes, meals and coffee breaks to social events etc. Moreover, all the participants stay in the same hotel near the University of Zürich, which not only makes it convenient for getting to class on time, but also gives you the opportunity to socialize with other participants. To spend almost two weeks day and night with a group of people definitely creates new friendships that will last long after you say your goodbyes.

To be given the opportunity to be a part of the 2019 Zürich School of Crystallography not only enriched my understanding of crystallography, from which I will most definitely benefit in my professional field, but also gave me the chance to meet some amazing people who made my stay truly unforgettable.

MEETING REPORT

International Summer School of Crystallography 2019 – Fundamentals of Crystallography

Wolfgang Brehm



The International Summer School of Crystallography 2019 – Fundamentals of Crystallography (ISSC19) took place in Hamburg, Germany, from 2 to 8 June 2019, following the format of the previous school in 2016. There were 34 students from Europe and abroad that took part, filling all the available spots.

The lecture series on the fundamentals of crystallography – symmetry, space groups, Fourier transforms, diffraction – presented by Carmelo Giacovazzo was supplemented by talks from Arwen Pearson, Professor Henry Chapman, Kay Diederichs, Thomas White and Pablo Bereciartua Perez. The additional talks expanded the scope to applied methods and statistics, and generalized the previously presented concepts. This provided prospects for practical applications and additional motivation.

During the lectures and the short exercises there was time for discussion and questions from the students. Many students stayed long after the lectures and the talks to interact with the speakers, who were happy to try and help them with their scientific problems.

There was some time for social events, which the students used to network and relax. The barbecue on the first day brought everyone together to get to know each other. On Wednesday afternoon we visited FLASH (a free-electron laser), REGAE (a relativistic electron gun for atomic exploration) and PETRA (a

positron–electron tandem-ring facility) on the DESY (Deutsches Elektronen-Synchrotron) premises and took a harbour boat trip, which was widely enjoyed.

At the end of the course, the participants filled in an evaluation form. The responses were largely positive and the feedback indicates that they are much more informed about the fundamentals of crystallography thanks to the course. Based on the feedback, we concluded that the three-year hiatus was too long and that the school should ideally be held every two years.

MEETING REPORT

27th Slovenian-Croatian Crystallographic Meeting

Marta Počkaj



Plenary lecturers, from left: Matic Lozinšek, Petra Bombicz, Martina Vrankić and Piero Macchi. (Photo by Krešimir Molčanov.)

The 27th Slovenian-Croatian/Croatian-Slovenian Crystallographic Meeting was held on 19–23 June 2019 at the Grand Hotel Sava in the town of Rogaška Slatina, Slovenia. There were 55 registered participants from Austria, Hungary, India, Italy, Switzerland, Ukraine, Croatia and Slovenia. Four plenary lectures were presented: *Synthon/property-engineering of calixarenes (supramolecular interactions, shape and symmetries)* by Petra Bombicz, Research Centre for Natural Sciences, Hungarian Academy of Sciences, Budapest, Hungary; *Are there molecules in crystals?* by Professor Piero Macchi, University of Bern, Switzerland; *Ambient and non-ambient driven X-ray powder diffraction: insights into the structure-property relationship in powders* by Martina Vrankić, Ruđer Bošković Institute Zagreb, Croatia; and *Noble-gas chemistry in the 21st century* by Matic Lozinšek, University of Ljubljana, Faculty of Chemistry and Chemical Technology & Jožef Stefan Institute, Slovenia.

One of the advantages of the Slovenian-Croatian meetings is that all participants give oral presentations, providing young scientists with the opportunity to present their work in a friendly but professional atmosphere. A total of 38 short oral presentations addressed contemporary topics in crystallography: structure determination of organic, inorganic and coordination compounds; crystal architecture and design; phase transitions, solid solutions, structure-property relationships, synergy of diffraction and complementary techniques; and history.

The meeting was co-organized by the Faculty of Chemistry and Chemical Technology, University of Ljubljana, and the Croatian Crystallographic Association under the auspices of the University of Ljubljana and promoted by the Slovenian Chemical Society. There was no registration fee; therefore, we thank the sponsors, donors and advertisers: Renacon, Rigaku, Bruker, Crystal Impact, Dectris, Optik Instruments, Aparatura, Lek-Sandoz, Krka and Scan.

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

FEATURE ARTICLE

Crystallography in the movies

Mike Glazer



A few years ago, Immediate Past President of the IUCr, Marvin Hackert, drew my attention to a Hollywood movie in which the word "crystallography" is mentioned. The movie in question is "[No Highway in the Sky](#)", made in Britain in 1951 by 20th Century Fox, and can be seen, for example, [here](#). The film stars, amongst others, the famous Hollywood actors James Stewart and Marlene Dietrich.

James Stewart plays the part of an aeronautical engineer involved in the design of a new type of aircraft, but he discovers that there is a possible fault in the design that would be catastrophic for the safety of the aircraft. Of course, he is rebuffed by his employers, but to determine if he is correct he takes a flight in the new aircraft along with other passengers, including Marlene Dietrich. The story is rather prescient in that three years later there were catastrophic crashes of the first jet airliner, the de Havilland Comet, caused by structural failure. Anyway, during the flight there is a short scene between Stewart and Dietrich in which they are having a conversation. I had wanted to include a clip here, but on contacting 20th Century Fox, I found that they wanted payment amounting to several thousand dollars (a bit out of the IUCr's league)! Fortunately, however, I have found the relevant clip on YouTube

and the important part for our purposes is at 1:28 minutes into the clip. For convenience, I have written out below a transcript of the conversation between Stewart and Dietrich here:

MD: Haven't you any family?

JS: Yes, I have Elspeth. That's my little girl.

MD: That's quite a lot to come back to.

JS: Oh yes. Why, that didn't mean I wouldn't like to. We are really very fond of one another. But, but I've been thinking about that. And... she's 12 now. Her character has formed, I think. Mary did that, mostly. She,... that's my wife. I wish it didn't have to be like that. But she's developed to such a point I think she is going to be alright. Of course, I haven't been able to help in a lot of things. She is much more soundly developed than most children her age. She really has a remarkable grasp of crystallography.

MD: Oh, that's very good of course. [pause] What is it?

JS: Well, it's quite fundamental. It's always been odd to me that the schools don't teach it.

I love that last line! Now, this is quite remarkable, as the discussion between them really has nothing to do with the rest of the film. There must have been a reason for inserting this into this film, but why?

The clue, I think, is in the date and place of production, 1951. Because of the Second World War, which ended in 1945, Britain was in a severe state of depression. The country owed a huge amount of money and there were still areas of bombed sites. The government at the time decided that in order to lift the spirits of the country they would hold a national festival, 100 years after the Great Exhibition of 1851. Most of the new festival would take place on the South Bank of the River Thames in London, where all that is left today is the Festival Hall. This was called the Festival of Britain, and was intended to showcase all the latest in science and technology, pointing to a glorious future. I recall as a child of 8 years the excitement of going to see it. The Festival was intended to restore Britain's faith in itself as a productive industrial nation after the ravages of World War Two, to promote better and more practical design in the rebuilding of the country's towns and cities, and to celebrate innovation in British architecture, design, industry and the arts. More than 8.5 million people visited the Festival's newly developed main site on London's South Bank – those that came to dine at the event's Regatta Restaurant were exposed to textile and furnishing patterns that came from a hitherto unexplored source: the molecular-scale images of X-ray crystallography.



Figure 1. Helen Megaw, queen of the perovskite structure.

The crystallographer Helen Megaw (Figure 1), in 1946 at Birkbeck College, London, and later the Cavendish Laboratory, Cambridge, had the marvellous idea of suggesting crystallographic designs to the Director of the Design Research Unit: "I should like to ask designers of wallpapers and fabrics to look at the patterns made available by X-ray crystallography. I am constantly being impressed by the beauty of the designs which crop up." This later led to the formation of the Festival Pattern Group. With the cooperation of Lawrence Bragg, Kathleen Lonsdale, Dorothy Hodgkin and others many designs were suggested to be used as curtains, carpets, restaurant items etc. Helen Megaw was officially invited to act as scientific consultant in August 1949. The result was that throughout the Festival site, many designs based on crystallography appeared. Some examples are shown in Figures 2 and 3.



(a)



(b)

Figure 2. (a) Cloth with design based on Megaw's afwillite structure. (b) Tie based on Dorothy Hodgkin's insulin structure.



(a)



(b)



(c)

Figure 3. (a) The Regatta Restaurant at the Festival of Britain showing several crystallographic designs. (b) Cups and saucers. (c) Menus.

Out of interest, you can find many web pages, including film shots, that describe the Festival, for example

<https://www.historic-uk.com/HistoryUK/HistoryofBritain/The-Festival-of-Britain-1951/>

<https://www.youtube.com/watch?reload=9&v=m9uGlfvyH0M>

<https://www.vam.ac.uk/articles/the-festival-of-britain>.

It seemed that crystallography was the "in" science of the time pointing to the future. After the Festival closed most of the design materials were lost but then eventually rediscovered and exhibited in 2008. I believe that many of them are now in the Victoria and Albert Museum in London. If you would like to learn more about crystallography and the Festival of Britain, I can strongly recommend getting hold of the beautiful book *From Atoms to Patterns* by Lesley Jackson.

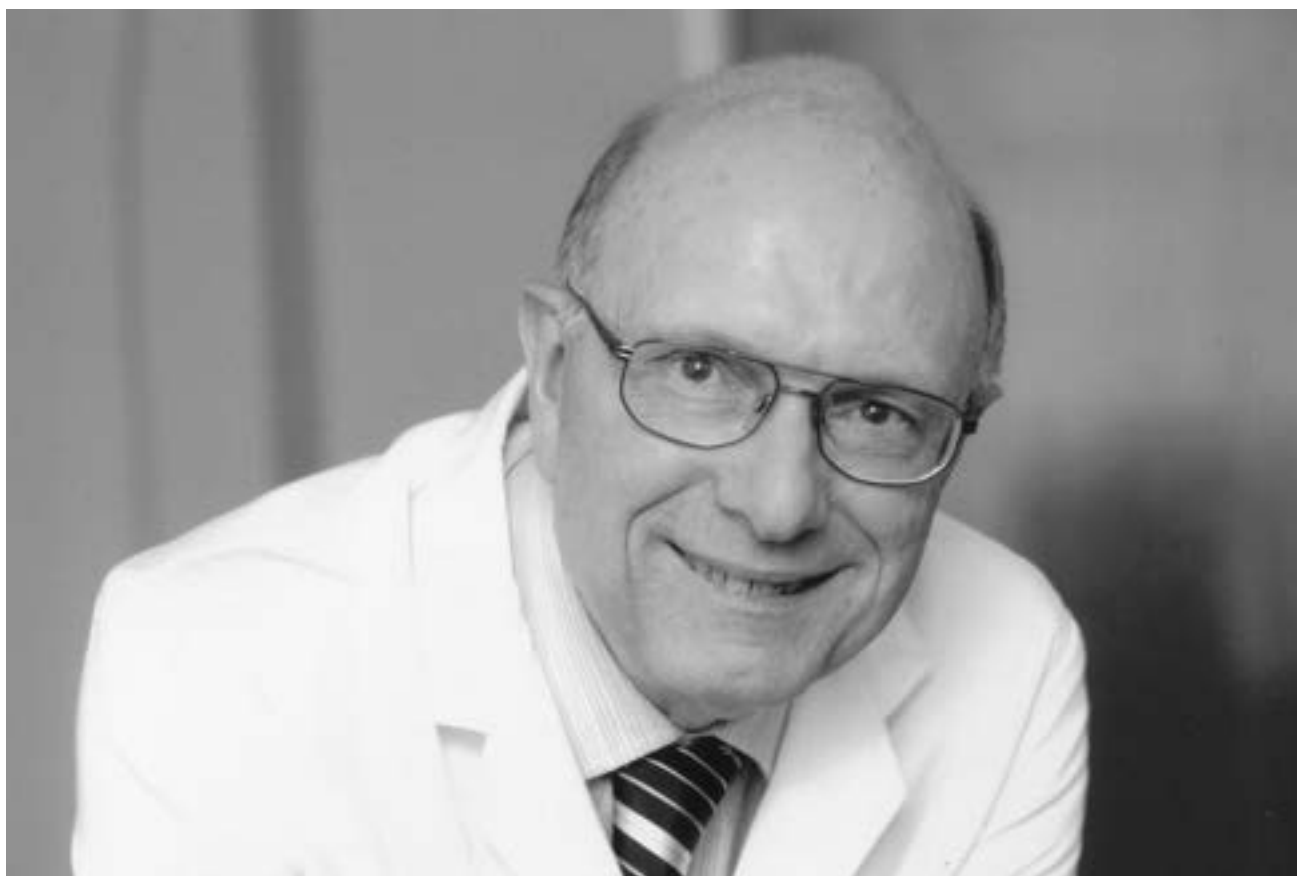
So, going back to the movie, I can well imagine that the producers or the director at the time, filming near London, must have been well aware of the Festival of Britain during that summer of 1951, and, I assume, decided to add a comment. I do wonder if perhaps Helen or another crystallographer might have mentioned this to the movie makers.

If you know any other examples of crystallography in the movies, [do let me know](#).

OBITUARY

Carl Schwalbe (1942-2019)

Simon J. ColesJohn R. Helliwell



Carl Schwalbe was known to so many of us in the global crystallography community. A large number of you will remember having met him personally at one of the many conferences he attended, as he was a regular at IUCr Congresses and ACA, ECA, DGK and BCA meetings. In the last decade he enjoyed these meetings as a retiree from an academic job, but not from the academic life and community.

It was during this time that he very seamlessly, competently and uncomplainingly carried out the role of Editor of the BCA quarterly magazine, *Crystallography News* – the membership of this organisation will be forever indebted for this service. Through his many meeting reports Carl kept a large number of BCA members aware of proceedings around the world. His accounts were not only of the academic sessions; he was always to be seen socialising at the commercial exhibitions, coffee breaks and conference dinners and had a delightful and insightful way of reporting these too! In this capacity Carl also attended the International Year of Crystallography launch event in Paris, held at UNESCO, in January 2014 and accordingly wrote a comprehensive report in the [March 2014 edition of *Crystallography News*](#) (pp. 12–14). It was always enlightening to read Carl's Editorials for *Crystallography News* – they were absorbing, humorous and could be on almost any topic imaginable! For example, Carl's March 2018 Editorial contained the following anecdote within a piece aimed at encouraging readers to attend more conferences!

"Two other meetings should inspire you to put fingers to keyboard and dash off a couple of brilliant abstracts. (When I started in crystallography, I'd have said "put pen to paper". I suppose some of you will now put fingers to touchscreen. I still wince slightly when I do this, remembering

how I used to tell off my students when they touched the screen of my precious Silicon Graphics workstation with greasy fingers.)”

Carl grew up in Ohio, USA, after which his academic path was as follows:

1959–1964 Chemistry (*summa cum laude*), Oberlin College, OH, USA;

1965–1970 PhD, Harvard University, Cambridge, MA, USA (PI, Professor William N. Lipscomb);

1970–1972 Research Fellow, Max Planck Institute for Experimental Medicine, Göttingen, Germany (PI, Professor W. Saenger);

1972–2019 Lecturer, Senior Lecturer, Professor, Emeritus Professor in Medicinal Chemistry, Aston University, UK;

2010–2019 Emeritus Research Fellow, Cambridge Crystallographic Data Centre (CCDC), UK.

Carl’s depositions in the CCDC ranged from EAMBNO10 first published in 1971 to XEZFIU, his most recent, published in 2018. His most cited article [Chattopadhyay, D., Chattopadhyay, S. K., Lowe, P. R., Schwalbe, C. H., Mazumder, S. K., Rana, A. & Ghosh, S. (1993). *J. Chem. Soc. Dalton Trans.* 913–916, “Synthesis and structural studies of tetraaquacopper(II) diaquabis(malonato)cuprate(II)” with 72 citations] featured the crystal structure PECMIT.

Carl was truly a member of the worldwide crystallographic community and in his IUCr *World Directory of Crystallographers* entry he identified his research interests as chemical crystallography, drug design, hydrogen bonding, molecular modelling, molecular recognition, drugs and MO calculations. Besides presenting his research at various of the IUCr Congresses, Carl published extensively in IUCr Journals including 32 *Acta Cryst. C* papers, 6 in *Acta Cryst. B*, 1 in *J. Appl. Cryst.* and 19 in *Acta Cryst. A*. A more detailed list of Carl’s publications is available at his [University of Aston legacy web page](#). Carl was to have lectured at the [IUCr Committee on Data Workshop](#) at ECM32 in Vienna, Austria, in August 2019. Instead Simon Coles and Suzanna Ward presented his latest work and ideas on the challenges of correct tautomer determination. This research was undertaken by Carl as a Cambridge Crystallographic Data Centre Honorary Fellow and led to questions of how best to remediate those cases held in the Cambridge Structural Database as described in his article Schwalbe, C. H. (2018). *Crystallogr. Rev.* **24**, 217–235.

The BCA will publish a more comprehensive obituary honouring Carl’s contributions to our community in the December 2019 issue of *Crystallography News*, which is also available [here](#).

Carl will be very much missed – most definitely by his readers but also by many in the international crystallographic community.

IUCR SUPPORTED EVENTS

IUCr supported meetings

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



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

Skukuza, Kruger National
Park, South Africa



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

Nairobi, Kenya

MEETINGS CALENDAR

Meetings calendar

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

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