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President's Letter – Winter 2023

Santiago García-Granda

I am writing this letter as we are in the midst of the Christmas season, as we are about to close the year 2023, which marked our 75th anniversary as a scientific organisation, and as we are about to begin 2024.

In the years between IUCr Congresses, 2024 and 2025, the spotlight should be aimed at our Regional Associates, ACA, AfCA, AsCA, ECA and LACA, all of which have announced their next meetings. This will be a wonderful opportunity to take the pulse of the state of crystallography and structural science at a regional level and also to establish new bilateral and multilateral connections between the Regional Associates and the National Committees. The IUCr, through its Meetings Support Committee, is doing its best to facilitate the participation of young scientists and to have the maximum prominence in these meetings and often associated schools. Our journals are very interested in the contributions arising from these meetings.

The calls for nominations for our flagship Ewald, Bragg and Struchkov Prizes are coming soon. The Union makes a significant financial effort to recognise the careers of the most brilliant crystallographers and structural scientists at various stages of their careers, and it is very necessary for us to be able to identify the best candidates in all scientific areas, particularly women. Therefore I ask for your collaboration with the Selection Committees in nominating candidates to ensure that the awardees are the best possible representation of our excellence and our diversity.

The IUCr Committees and Commissions, once consolidated after the renewal of their members approved by the 26th General Assembly in Melbourne, will be renewing their activity in the various scientific and organisational areas that constitute the heart of our Union and that set the guidelines for our future scientific developments. At the moment, all our Commissions are working at a good pace with the autonomy that characterises their mode of operation within the framework of the IUCr, according to the updated guidelines.

Our ten scientific journals and International Tables, together with this Newsletter and the other IUCr publications, provide the image of both our scientific level and our social contribution. They also provide us with the necessary financial return to maintain our functioning and the patrimony of our activities in order to promote the development of crystallography and structural science in the most economically and academic disadvantaged areas and to ensure the generational renewal of our scientific community.

The new members of the Executive Committee have organised their visits to our office in Chester to familiarise themselves with the activity of the 24 people who constitute the stable nucleus that efficiently carries out our technical and administrative work, essential for the functioning of the IUCr. Also, this group is very conditioned by the inevitable generational handover, for which – under the supervision of our Finance and Executive Committees – the IUCr CEO, Dr Alex Stanley, must plan with a vision for the future.

It was good for the new General Secretary and Treasurer, Professor Trevor Forsyth, and me to meet many of our team in Chester and see the initiatives being implemented to make publishing in our journals more attractive and make our journals more competitive. We also need the help of our scientific Commissions and our Regional Associates and National Committees to convince every scientist to publish their best contributions in IUCr journals. I consider that it is especially important for us to make it easy for young people to make their first scientific contributions to our journals and encourage them to transmit their comments through our Newsletter and social networks.

Trevor's role must be decisive in the configuration of the working teams and in the control of the activity of the Chester office and in the control of the finances and resources of the Union. This intention framed our recent working visit to Chester, on 27 and 28 November, where we met with Professor Malcolm Cooper, the Convener of the IUCr Finance Committee, as well as Alex and Peter Strickland, Executive Managing Editor, visiting the

different sections of the office and noting the technical and administrative improvements underway, as well as the various threats to the Union.

I would like to remember, emotionally and gratefully, those who left us in 2023 and send a message of appreciation to their families, colleagues and friends. I would also like to welcome those who joined the IUCr, either via their National Committees or as members of the IUCr Associates Programme. I do not want to forget our industrial partners, who are so supportive of our meetings and schools with their financial and technical contributions. Thank you very much for being an important part of the IUCr family.

The process initiated in Melbourne to define our Purpose, Vision and Values in an open and participatory way, to ensure the scientific and social leadership of crystallography and structural science for the remainder of the 21st century, is advancing according to the planned steps until being approved by the 27th General Assembly in Calgary in 2026. A survey to gather the opinion of the global IUCr community has recently been conducted to concretise the ideas that best define our identity and our objectives. The results will be presented to the entire community once they have been analysed by the Executive Committee.

The Executive Committee, which had its first virtual bimonthly meeting on 7 November and has another planned for 9 January, will meet in person in Denver, CO, USA, in July 2024, coinciding with the ACA's annual meeting. The Finance Committee meeting will be held at the same place in the preceding days. Prior to that, in March, we will have the spring meetings of the Journal Management Board in Chester and the Finance Committee in Lund, Sweden.

The Executive Committee, through its President or some of its members, will try to be present, representing the IUCr, at the most important regional and international events for the IUCr.

Our representative in the International Science Council (ISC), Dr Hanna Dabkowska, has reported on the approval process of the new ISC statutes, which, after intense activity by the International Unions, are proposed with an important protagonism of the International Unions in the decision-making processes of the Organisation. This is good news that we hope will be confirmed in the coming months.

The collaborative projects being developed with governments, companies and non-governmental organisations will give an extraordinary boost to the development of science in all regions of the world. The Africa Initiative, led by Professor Claude Lecomte, is achieving important results, and other activities in Kenya, led by Professor JuanMa García-Ruiz, with important local support, are in progress. The worldwide 2023 IUCr Crystal growing competition for schoolchildren is also in progress. The development of new infrastructures in less developed countries and the project Light Sources for Africa, the Americas, Asia and the Middle East Project (LAAAMP) are going well. And the International Year of Basic Sciences for Sustainable Development, now drawing to a close, has served as a prelude to the International Decade of Sciences for Sustainable Development 2024–2032 (IDSSD).

In this time of serious and bloody international conflicts and natural disasters, many of them due to the climate change that our societies are causing, global scientific societies must be able to identify their role in building a better world for future generations, based on scientific, technical and humanistic knowledge. As expressed before, our role is to promote, defend and protect science and scientist, keep ourselves out of fanaticism of any kind, by maintaining the bonds of scientific collaboration above conflicts and align ourselves with the progress of global society in terms of peace, justice and equity, diversity and sustainability. We have to ensure that future generations have open minds, global awareness and the resources and conditions to sustain a better and better life on the planet, and this is not only for the human species but also to maintain the planet's biodiversity and wildlife.

Once again, many thanks to all those who form and make our organisation work, the Regional Associates, the IUCr Commissions and Committees, Editors, Co-editors, referees and authors of our journals, our Chester staff, and all individual crystallographers, women and men.

Thanks to IUCr Newsletter Editor Mike Glazer, his team and all contributors.

Many thanks to all for keeping the IUCr alive, active, strong and human.

Merry Christmas and Happy 2024 from all of us!

Editorial

Mike Glazer

The IUCr Congress this summer was a great success, with attendees coming from across the world. Bringing school children into the heart of a scientific congress such as this was brilliant. Stuart Batten, Helen Maynard-Casely, Rosemary Young, Emily Furlong and Bryce Mullens (ref) describe this aspect of the IUCr Congress entitled Crystal-a-con. We are indeed fortunate that crystallography and crystal structures can be made to look so attractive and interesting to excite the interest of young people.

The science of crystallography has a long history, but it is only within the last 400 years or so that our understanding of crystals and their atomic structures has “crystallised”, so to speak. The study of crystallography turns out to have been conducted by many scientists well known for their research into other scientific disciplines. So, for example, Johannes Kepler, famous for his theory of planetary motions, also became interested in the symmetry of snowflakes and also in the close packing of spheres to explain morphology. Then again, Robert Hooke, famous for his Law, among other things, also tried to explain crystal morphology using the packing of spheres. So, the principle of periodicity in crystals was the subject of interest for many scientists in the past. One of my scientific heroes, Louis Pasteur, better known for his work on microbes, also started off as a crystallographer with his study of optical activity in tartrate crystals. So, now I see that even John Dalton, whom we all know for his theories on gases and atoms, also had crystallographic leanings. I never knew that, did you? Well, in a feature article, Istvan and Magdolna Hargittai (ref) reveal all about this aspect of Dalton’s life.

From Robert Hooke's *Micrographia* (1665). The lower diagram is for crystals grown from urine.

One of the problems facing crystallographic publications is how to evaluate the correctness of a particular submitted crystal structure. So, it is incumbent on all referees and journal editors to ensure that at least the proposed structure makes chemical sense. In my experience, there are two or three cases that need attention. Sometimes, it is a matter of fraud. For example, recently, I refereed a paper in which it became evident that the authors had merely copied the coordinates from a much earlier Rietveld refinement published by other scientists and used them with the atom labels changed to match those in their own compound of interest. Then, you have cases of scientific misunderstanding. I am reminded that several years ago, I came close to failing a Ph.D. student during his viva voce examination (something that I had never done before) over his quoting of errors in pressure measurements to 7 figures of decimals! Even after explaining that you cannot simply copy out the results of a computer calculation like that, and after he tried to argue that the computer results are correct, he finally agreed to change the errors in his thesis to single figures of decimals, but he did with exceedingly bad grace. I don't think he ever really understood my objection despite nearly an hour of trying to explain to him the significance of errors.

The article on mythical compounds (ref) highlights problems with structure validation. It is all too easy to collect some data and refine it to apparently good agreement but arrive at a nonsensical crystal structure arrangement. A personal example of this was when I had a paper to referee in which the authors claimed to have carried out a Rietveld refinement on both X-ray and neutron powder data and to have obtained very low, so-called R-factors. However, they did not give the actual refined atomic coordinates in a table. When they finally revised the paper, I saw that their x-ray and neutron coordinates bore no resemblance to each other. On plotting out their structures, it became obvious that the refined structures made no sense at all! Perhaps an extreme example of mythical compounds has been in the recent publication in *Nature* of the use of generative AI to predict the existence of hundreds and thousands of new crystal structures. Unfortunately, as pointed out in the Twittersphere (or is it X-sphere?) by Robert Palgrave, examination of the structures reveals that many seem to make no chemical sense at all nor provide powder diffraction patterns that do not match the experimental measurements! Computers, eh?

Sadly, as usual, we have to report the deaths of two of our distinguished colleagues, Bob Blessing (USA) (ref) and Henk Schenk (Netherlands) (ref). Both were well known for their scientific research and their services to the crystallography community. I remember many happy discussions with Henk on the crystallography of chocolate, which turns out to be the most essential factor in determining its taste and texture. Crystallography appears everywhere!

JOHN DALTON REMEMBERED

Istvan Hargittai and Magdolna Hargittai

John Dalton was a pioneer in modern science. Whenever his name is mentioned, we think, among others, of his atomic theory and color blindness ("Daltonism") but seldom of his contribution to crystallography. His ideas about packing in water and in ice were most forward-looking.

When in the years 1983–1985 we were working on our book *Symmetry through the Eyes of a Chemist* in English (its first edition) [1], we found the development of the ideas of dense packing most fascinating. This was something that had hardly interested us before because our principal research was in gas-phase molecular structures where packing was not a subject of consideration. After Lucretius and Johannes Kepler, we enjoyed Dorothy Hodgkin's essay "Moments of Discovery," referring to the crystallographer John Dalton in a collection of papers in *Kristallografiya* honoring Boris K. Vainshtein [2].

Fig. 1 Dalton's models for water (1 and 3) and for ice (2, 4, 5, and 6) in his book *A New System of Chemical Philosophy* ([3], p. 128, plate III)

Hodgkin called attention to the remarkable difference between the packings in liquid water and ice manifested in Dalton's 1808 treatise (Figure 1). Dalton's idea was that the building elements in solid ice are more densely packed than in liquid water. Hodgkin showed the reappearance of Dalton's ideas in the model of the atomic arrangement in the 2Zn-insulin crystal [2]. The molecular structure of insulin is very complicated, but the molecular packing, especially the arrangement of the insulin hexamers, reminded her of Dalton's hexagonal ice.

Fig. 2 Closely packed spheres by Dalton [4]

Fig. 3 Closely packed cannon balls in the Castel Sant' Angelo, Rome (photograph by the authors)

In the third edition of our *Symmetry through the Eyes of a Chemist* [5], we included another representation of the close packing of spheres from John Dalton (Figure 2) [4] and a photograph of a close-packed arrangement of cannon balls (Figure 3) ([5], p. 422).

Fig. 4 A well-known engraved portrait of John Dalton by W. H. Worthington, 1823, after J. Allen, 1814 (Wellcome Collection)

Fig. 5 John Dalton's mezzotint portrait by C. Turner, 1834, after J. Lonsdale (Wellcome Collection)

John Dalton's (1766–1844, Figures 4 and 5) oeuvre has been treated extensively in the literature and in chemistry texts. We single out the monograph by William C. Henry, which appeared in 1854 and is accessible freely on the Internet [6]. Following a brief biographical introduction ([7], p. 106), we present a sampler of memorials to John Dalton in the remainder of this communication. It is far from complete and is meant to indicate his international recognition.

Fig. 6 John Dalton's memorial plaque at his birthplace in Eaglesfield (photograph by Graham Robson, reproduced under the Creative Commons Attribution-ShareAlike 2.0 license). There is a similar plaque on the wall of the Ape and Apple pub on John Dalton Street in Manchester. Yet another Dalton memorial plaque is on the wall in the offices of the Manchester Literary and Philosophical Society. Dalton was its president from 1816–1844

Dalton was born in Eaglesfield in Cumberland, England (Figure 6). His parents could not afford to give him a formal education, but he was precocious in self-study, and already at the age of 12, he was teaching at a

village school. This was followed by a series of teaching positions and sometimes even school principal positions. He landed a tutorship in mathematics and philosophy in 1793 at the New College of Manchester. It was about this time that he published his first book on meteorology. Other books followed, including one on the familial condition of color blindness, eventually called "Daltonism."

He investigated the properties of gases and discovered the Law of Partial Pressures. He is best known for his atomic theory and his charts of atomic weights. He described his theoretical findings in his *A New System of Chemical Philosophy*, published in 1808 and appended in 1810. His theoretical discoveries helped the chemical industry establish the correct proportions of the component elements in the compounds being produced.

He was a Quaker, and his modesty made him decline the Fellowship of the Royal Society; although C. Turner's portrait says, "Dr. DALTON, F.R.S." Dalton accepted an honorary doctorate from Oxford University.

Fig. 7 Statue of John Dalton by Francis Chantrey, 1838, Manchester Town Hall (photograph by the authors)

It was a great distinction that in 1838, his statue was created by the distinguished sculptor Francis Chantrey (1781–1841). It now stands in the Manchester Town Hall (Figure 7), opposite James Prescott Joule's (1818–1889) statue by Sir Alfred Gilbert. It is most appropriate to have the memorials of these two giants of science close to each other as the elderly Dalton was a mentor of the young Joule.

Fig. 8 Stone portrait of John Dalton on the back façade of the former I.C.I. building, Smith Square, London SW1P (photograph by the authors)

Imperial Chemical Industries's (I.C.I.) headquarters was opened in 1929 after I.C.I. was formed because of the merger of several companies. I.C.I. left the site in the 1990s following the restructuring of the company giant. 11 stone portraits of distinguished chemists decorate the façades of the former headquarters. Four of them were directly associated with I.C.I. or its predecessor companies: Harry McGowen, Alfred Nobel, Ludwig Mond, and Alfred Mond. The other seven were great contributors to chemistry: Joseph Priestley, Henry Cavendish, Antoine Lavoisier, John Dalton (Fig. 8), Justus von Liebig, Marcellin Berthelot, and Dmitri I. Mendeleev. Our guidebook, *Science in London*, describes the exact location of these stone portraits on the three segments of the façade [7] (pp. 103–110 and 240).

John Dalton's portrait, as an oil painting by Thomas Phillips in 1835, is one of many scientists' portraits, in the 300,000-strong collection of the National Portrait Gallery in London, at St Martin's Place, WC2H. The Gallery has been at this location since 1896, but the collection first opened in 1856.

Fig. 9 John Dalton as a low-relief statue on one of the six panels on the front façade of the headquarters of the U. S. National Academy of Sciences (photographs by the authors)

The United States Congress chartered the National Academy of Sciences of the U.S.A. (N.A.S.) as an independent institution in 1863 during the American Civil War. Its headquarters were located for a long time at the Smithsonian Institution. Its current headquarters opened in 1924 at 2101 Constitution Avenue N.W. There are six low-relief bronze panels by the sculptor Lee Lawrie located between the windows on the front façade of the headquarters. Three panels are left from the entrance and three are right from the entrance. Each panel depicts six scientists (except the middle right, which depicts seven). John Dalton is on the middle-left panel, which displays the following scientists: Humboldt, Dalton, Lamarck, Watt, Franklin, and Huygens (Figure 9). More about the decorations, including these panels, of the headquarters of N.A.S. can be found in [8].

Two bas-relief portraits of John Dalton. Left: Fig. 10 On the façade of Olive Tjaden Hall at Cornell University, Ithaca, New York. Right: Fig. 11 On the wall of the entrance lobby to the Ceremonial Hall of the tower building, Lomonosov Moscow State University, one among 24 mosaic portraits of Russian and international scientists [9]. Both photographs by the authors.

Two bas-relief portraits of John Dalton in Budapest. Left: Fig. 12 On the Trefort Campus of Eötvös University, in the building that was first erected for chemistry in 1871. Today, this is part of the Faculty for Humanities ([10], pp. 65–66). Right: Fig. 13 On the campus of the Veterinary School ([10], p. 142). Both photographs by the authors.

The above four bas-relief portraits (Figures 10–13) expand the international outlook of our collection of Dalton memorials but should be considered only as accidental examples that must be a small fraction of Dalton memorials worldwide. The present communication also exemplifies that Dalton's legacy belongs to broader domains in science than how his name is usually associated.

We conclude our presentation with an unusual group picture in which Dalton is depicted as one of the central figures in a large group of scientists and technologists.

Fig. 14 "Distinguished British men of science 1807–1808 assembled in the library of the Royal Institution, London. Mezzotint by W. Walker and G. Zobel after F. Skill and W. Walker, ca. 1860, after Sir J. Gilbert" (Wellcome Collection)

Fig. 15 A key to the identities of the sitters on Fig. 16 (Wellcome Collection)

This image of Figure 14 has quite some literature (see, e.g., [11 and 12]). There are over fifty men in this image. Careful examination by a science historian has shown that they could never have come together as a group, and the meeting could not have taken place at the Royal Institution. Many distinguished scientists and technologists are in the picture, but many other important scientists are missing, especially in biology, which is hardly represented. The portraits of those presented were copied from other works of art. Thus, Dalton's portrait closely resembles W. H. Worthington's 1823 engraved Dalton portrait (see Fig. 4 above) with a few minor alterations. The identity of those in Figure 14 can be determined from the key given in Figure 15. The period, 1807–1808, was George III's reign, who himself was a scientist, although, alas, eventually his mental state prevented continuation of his royal duties. An attractive indication of the popularity of the pioneers of science and technology during the Victorian era was that copies of this group image were available for purchase. Prints of different quality were produced, and they were priced accordingly.

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The International Tables Symmetry Database – a comprehensive guide

Author not stated in source

The International Tables Symmetry Database, part of International Tables for Crystallography, is a collection of individual databases of crystallographic space-group and point-group information. Programs are provided to access and interactively visualize the data, and also allow new data to be calculated 'on the fly', facilitating the in-depth study of group– subgroup relations, domain structures and twinning, families of related crystal structures and phase transitions, and the prediction of new crystal structures. The Symmetry Database has been available since 2021 [OK or earlier?] to subscribers to the online version of International Tables for Crystallography.

In a highly informative open-access article in the Teaching and Education section of the latest issue of the Journal of Applied Crystallography, Gemma de la Flor, Eli Kroumova, Robert M. Hanson and Mois I. Aroyo present the server-side crystallographic programs and interactive visualizers of the Symmetry Database and provide examples showing how they can be used.

An appendix to the article, based on information from the Teaching Edition of International Tables for Crystallography and International Tables for Crystallography Volume A, provides some basic definitions and explanations of the notation used in the description of symmetry operations, coordinate transformations, and subgroups and supergroups of space groups.

We strongly urge you to read this comprehensive guide to the many different features and uses of this unique resource.

Exploring tetrel bonding: a special issue of Acta Cryst. C

Author not stated in source

A snapshot of current progress in the field of halogen bonds, chalcogen bonds, pnictogen bonds, tetrel bonds and other σ -hole interactions appears on the cover of the special issue. Illustration courtesy of Brammer et al. Halogen bonding and related intermolecular (and sometimes intramolecular) interactions in which p-block elements in groups other than Group 17 serve in a Lewis acidic role have been and continue to be extensively investigated. Their applicability in supramolecular assembly is similarly well studied, with numerous reports of applications in crystal engineering, molecular recognition, catalysis, polymers and soft matter, materials chemistry, structural biology and medicinal chemistry.

This virtual special issue of Acta Crystallographica Section C: Structural Chemistry, titled "Halogen, chalcogen, pnictogen and tetrel bonds: structural chemistry and beyond", brings together 12 articles that cover a variety of aspects associated with halogen, chalcogen, pnictogen and tetrel bonds. The issue is introduced by a review by the Guest Editors, Lee Brammer, Anssi Peuronen and Thomas M. Roseveare. In "Halogen bonds, chalcogen bonds, pnictogen bonds, tetrel bonds and other σ -hole interactions: a snapshot of current progress", they present a compilation of review articles on σ -hole interactions published since 2013 alongside an overview of the 11 articles in the special issue on this topic.

There are articles that focus on structure, bonding and bond strength, articles that investigate co-operation or competition between different classes of interactions and articles that explore the relationship between these interactions and chemical or physical properties of the compounds and materials involved. Although all articles involve characterization by single-crystal X-ray diffraction, a number have a prominent focus on other experimental techniques or are combined with interpretation from theoretical calculations. Halogen bonding and chalcogen bonding dominate these articles, consistent with the wider literature.

Crystal-a-con at IUCr 2023

Stuart R. Batten, Helen E. Maynard-Casely, Rosemary J. Young, Emily J. Furlong and Bryce G. Mullens

How many times in your career have the world's crystallographers gathered in your town (or even your country when you are in the Southern Hemisphere)? From the point that the SCANZ team won the bid to hold the 26th IUCr Congress in Melbourne, we realised that this was truly a once-in-a-lifetime opportunity to push communication of crystallography beyond the Brillouin zone. And so, the Bragg Your Pattern project (<http://braggyourpattern.com>) was formed!

The Bragg Your Pattern committee proudly wearing the popular Bragg T-shirts specially commissioned for the conference (available still from <https://meganleestudio.com/>). Photo: IUCr2023 Congress.

In Australia and New Zealand, there is a big emphasis on developing Science, Technology, Engineering and Mathematics (STEM) resources for students in high schools (aged 11 and above) but less on those younger. The Bragg Your Pattern team realised that, through patterns and symmetry and its very visual nature, crystallography is an ideal topic to target with a younger audience. We started the project in 2022 with a national pattern competition, where students were encouraged to 'make' or 'see' a pattern and send the image to us. Those who made it to IUCr2023 would have seen these images on our Giant Buckyball during the conference.

Bragg Your Pattern competition winner's art was displayed on our giant buckyball. Photo: S.R. Batten.

But the pattern competition was just our warm-up, with the big event planned for 2023 - a pop-up crystallographic science festival held right within the conference venue! We brought together crystallographic-inspired exhibits, but our big draw was the inclusion of seven interactive activities. The event, 'Crystal-a-con,' was marketed to schools and members of the public and held on Friday and Saturday during the congress. Each of the interactive activities was named after a crystal system, and each visitor was given a passport so that they could collect stamps from each one.

A completed Crystal-a-con passport. Photo: R.J. Young.

Our Cubic activity was perhaps our headline activity, and certainly, the one that attracted many IUCr delegates - trying to break the world record for the largest crystal structure model! The previous record (<https://guinnessworldrecords.com/world-records/109929-largest-sodium-chloride-molecular-structure-model>) was for a model of sodium chloride (common table salt) which contained 38,880 individual 'atoms' (though it has since been expanded to 42,875 atoms, <https://worldrecord.r-krickl.com/en/>, <https://www.facebook.com/worldrecordcrystalmodel>, <https://www.facebook.com/worldrecordcrystalmodel>).

In the weeks before the conference started, a number of smaller parts of the overall model were built by staff at the Australian Synchrotron. These pre-built parts were taken to the conference venue and assembled and added to by conference delegates over the first 5 days of the conference. School groups and members of the public who attended Crystal-a-con also helped build the big model.

The world-record Diamond attempt proved a popular networking spot for delegates of IUCr2023, as well as a big draw as an interactive activity during Crystal-a-con. Photo: Thomas Proffen.

The statistics of the final assembled model were impressive: 62,356 atoms were connected by 121,547 bonds (i.e., 183,903 individual components that had to be connected together). Total weight 341 kg, total volume 4.47 cubic metres. Dimensions were 3.69 m along the bottom triangular edges, 2.31 m along the top triangular edges, and 1.11 m in height.

The completed world-record Diamond model. Photo: S.R. Batten.

Our hexagonal activity was on the sweet side! Sweets and crystals are both amazing individually, but they are the best together! Participants in the hexagonal activity built their own crystal structure models out of jubes (Australian jelly sweets) and toothpicks, using over 25 kg of lollies and 10,000 toothpicks. Starting with a simple cubic crystal structure, it was quickly apparent that this model was quite brittle and weak. Adding another lolly

to make a body-centred cubic structure made a much stronger assembly. Enthusiastic kids continued on to make extended body-centred cubic and hexagonal structures.

This activity was an excellent conversation starter to talk about everyday crystals such as salt and sugar and how they are similar and different from crystals like diamonds and rubies. The different ways the same building blocks (jubes and toothpicks) could be constructed to make stronger or weaker assemblies could be directly related to the difference between diamonds and graphite.

Many kids worked together to combine their 'unit cells' to make larger and larger lolly 'crystallites', even making them colour-coordinated. This activity was very popular, although that may have been because they could eat their lollies after they finished building!

Celebrating the patterns of the world was the theme for the Trigonal activity, which brought together a range of patterns from different cultures and explored the maths behind them (with Dr Katherine Seaton). Not only were participants able to create their own inspired patterns, but we also got them thinking, "When is a pattern not a pattern?" by introducing the 'Einstein' shape that had taken the news by storm a few months previously. Visitors were also encouraged to vote if they thought the shape most resembled a hat or a shirt! As you can see in the picture, the shirt won!

Hat or Shirt? Crystal-a-con visitors were able to vote on what they thought the latest Einstein shape most looked like. Photo: H.E. Maynard-Casely.

Our Orthorhombic and Tetrahedral activities were run by some fantastic partners. The CCDC brought their 'Crystal detectives'

(<https://www.ccdc.cam.ac.uk/community/education-and-outreach/outreach/home-learning-activities/identikit-of-common-substances/>) activity that they had run at a number of science festivals. The Australian audience had a great time identifying common substances from crystal structures; through the link, anyone can try this at home, too. Added to this, ANSTO - custodians of the central facilities in Australia - dispatched a team from their Discovery Centre to run a diffraction demonstrating activity with lasers on the Friday, while the Saturday theme revolved around the periodic table.

In the Monoclinic activity, the Crystal-a-con participants had the opportunity to build their own virus model out of paper! Thanks to the RCSB Protein Data Bank, we had a very nice template that could be easily punched out of a piece of card and folded up to make a Zika Virus model. For those participants wanting more of a challenge, Protein Data Bank Japan provided instructions and paper to fold an origami virus, and Dr Daniel Eriksson was on hand to help people fold an icosahedral virus from a single piece of paper. The Protein Data Bank in Europe was also involved and provided beautiful images from their 2023 PDB Art calendar to display.

Our Triclinic or "Meet the Crystallographer" station allowed us to make the most of the amazing crystallographers who had travelled from the other side of the world to attend IUCr2023. We had 12 crystallographers volunteer to share their work with our participants over the 1.5 days. These crystallographers came from countries across the globe, including the UK, Uruguay, Germany, Canada, and of course, Australia. The Crystal-a-con participants were amazed to hear about all the fascinating work the crystallographers did and excited to take home Prof Jennifer Martin's "My Aunt is a Protein Crystal Scientist" book and goodies from the Diamond Synchrotron.

A big thanks goes to all who helped make Crystal-a-con a reality, including many staff at Australian Synchrotron who were invaluable support for the logistics. Photo: H.E. Maynard-Casely.

Along with the interactive activities, we gathered together a number of additional exhibits, from crystallographic-inspired fashion (thanks to Dr Irene Suarez-Martinez with her Stem and needles project <https://stemandneedles.com/>), to giant crystal structures that had first been commissioned for the International Year of crystallography in 2014. Overall we created a pop-up science museum!

The knitted neuraminidase - one of our giant crystal structures from 2014. Photo: R.J. Young

As icing on the cake, we organized a public lecture by Prof Jenny Martin, who shared why she loves crystallography. The lecture touched on Australia's strong connection to this wonderful science, the incredible women who work in the field, and the amazing scientific advances our community has enabled through sharing resources and knowledge.

Prof Jenny Martin signing copies of 'My Aunt is a Protein Crystal Scientist' after her public lecture. Photo: R.J. Young.

A big thanks goes to all who helped to make the event the success it was: our IUCr volunteers (sporting their red Bragg T-shirts), the synchrotron staff who tirelessly made diamond and were invaluable in the logistics, and the conference organisers who supported the whole endeavour. Thanks also to all the IUCr delegates who stopped by and put some carbon atoms together; the event was truly community-supported.

Overall, our Crystal-a-con event was visited by 480 school kids, teachers and their families, giving them a great insight into the importance of crystallography and what life looks like on the atomic scale.

What are our next steps? Our giant diamond model is now destined to be broken down into the individual kits and will be donated, along with a supporting booklet, to more than 1,000 primary schools all over Australia and New Zealand to inspire the next generation of scientists and crystallographers. Particular emphasis will be given to remote, rural, regional, and low-economic opportunity schools, which are typically under-resourced in the area of STEM and/or have limited access due to distance to other STEM-supporting outreach programs. Hopefully, this, and the fact that we now have a toolkit of activities to run around the country, will mean a long public outreach legacy for the IUCr2023 meeting.

73rd Annual Meeting of ACA: The Structural Science Society (ACA2023)

Anna Gardberg and Samantha Powell

The 73rd Annual Meeting of the American Crystallographic Association: The Structural Science Society was held in Baltimore, MD, USA, on the traditional ancestral lands of the Piscataway and the Susquehannock tribes. At both the opening and closing of the meeting, we respectfully acknowledged and honored all Indigenous communities—past, present, and future.

The scientific program spanned July 8-11, 2023, with associated workshops on July 7. The program consisted of 47 daytime scientific sessions, 2 evening sessions, 3 poster sessions, 5 workshops and a 3-minute thesis competition. In contrast to ACA2022, this meeting was offered entirely in-person. The meeting was well-attended, with over 500 registrants and over 160 workshop participants.

The scientific program opened with a keynote address from Sir Venki Ramakrishnan, whose lecture “My Adventures in the Ribosome” was a wide-ranging overview of his personal and professional journey, culminating in unraveling the ribosome’s structure, and concluding by relaying how newer structural methods such as cryo electron microscopy (cryoEM) are enabling us to tackle ever-harder structural problems. Expanding on that theme, the Transactions Symposium was entitled “From Atoms to Cells – Electron Microscopy for Structure Solution”.

The subsequent three days continued with 6 parallel tracks of scientific sessions as well as 3 poster sessions.

Other highlights of the meeting were the sessions on machine learning, AI, and related subjects that are very topical to our profession. As well, the evening “Would you publish this?” session featured both small-molecule and macromolecular entries, filled the venue, and proved one of the most convivial of the week.

This year’s program continued to demonstrate the relevance of our new name, ACA: The Structural Science Society. We saw many talks covering structural techniques outside of traditional crystallography, such as BioSAXS and SANS, and multi-modal experiments.

Sessions on cryoEM and related techniques such as cryo electron tomography (cryoET) and microcrystal electron diffraction (MicroED) were also prominent, being featured in the Transactions Symposium as well as 5 other sessions.

Details on this and future meetings can be found at www.acameeting.com. More information can be found at our social media accounts on X and Instagram @ACAxal, Facebook @AmerCrystalAssn or LinkedIn. In anticipation of an in-person meeting for 2024, please mark your calendars to join us July 7-11, 2024 in Denver, CO!

11th training course on symmetry and group theory, Tsukuba, Japan, July 2023

Prof. Noriyuki Igarashi

The training course on symmetry and group theory in Japan was launched in August 2014, immediately after the IUCr congress in Montreal, on the occasion of the International Year of Crystallography. The motivation was to compensate for the lack for basic crystallography training in University curricula, which results in serious obstacles in daily crystallographic work, when the investigator needs to interpret his results, navigate through the International Tables for Crystallography, and perform all the tasks that a black box cannot do for him.

The training course is hosted at the High Energy Accelerator Organization site in Tsukuba and is offered free of charge to all students and scientists in Japan who need basic training in crystallographic symmetry. It is sponsored by The Crystallographic Society of Japan and the Institute of Materials Structure Science of the High Energy Accelerator Organization, and supported by a number of Japanese scientific societies and associations. It benefits from the precious help of Ms. Yoshimi Takahashi, dedicated secretary in charge of all the logistic and contacts with participants.

The course spans five full days, with morning and afternoon lectures and exercises, and night sessions for questions and answers, discussion, support for the exercises. It is taught in its entirety by Prof. Massimo Nespolo, from the Université de Lorraine (France). The unexpected success of the first course convinced the organisers to repeat it twice a year (March, August) until 2017, moving then to a once-a-year frequency when it became an official Interdisciplinary Lecture of the Graduate University for Advanced Studies (Sokendai), which entered as co-sponsor.

The program of the training course starts from basic algebra to bring everybody to a common background, and goes through theory and practice of crystallographic point and space groups, with extensive exercises on the International Tables for Crystallography, crystallographic calculations, group-subgroup relations, normalizers, chirality, geometric derivation of reflection conditions, crystallographic orbits, symmetry aspects of phase transitions, with examples of derivative structures and construction of structural model of low-symmetry polymorphs from the high-symmetry polymorphs.

The course is entirely taught in Japanese. Because of the language difficulties met by foreign students willing to attend the lectures, an English version has been offered since 2019, but had to be interrupted because of the SARS-CoV-2 outbreak in 2020 and could be restarted only this year, after foreign students were again allowed to come and study in Japan. The Japanese course was suspended only in 2020; in 2021 it was offered in a hybrid form, before going back to on-site lectures in 2022.

An advanced course is offered periodically to those who have attended the basic course. The first advanced course was offered in 2016. The second advanced course, originally planned for 2020-2021, had to be postponed and was eventually realized this year, with a program centred on groupoids and chromatic symmetry.

The twelfth course is planned for July 2024, both in English and Japanese.

Photo 1: group photo of the 2023 Japanese basic course

Photo 2: group photo of the 2023 English basic course

Photo 3: group photo of the 2023 advanced course

Chair of the local organizing committee

Electron Crystallography School 2023

Laure Bourgeois, Hongyi Xu and Tatiana Gorelik

On 19-21 August 2023, the Monash Centre for Electron Microscopy (MCEM) hosted the Electron Crystallography School 2023 (ECS2023), as a satellite event to the 26th International Union of Crystallography (IUCr) Congress. The School was organised by the IUCr Commission on Electron Crystallography, with Hongyi Xu, Tatiana Gorelik, Mauro Gemmi and Laure Bourgeois as co-chairs. The ECS2023 focused on two broad topics that have seen considerable development in the last decade or so: 4D-scanning transmission electron microscopy (4D-STEM) and 3D/micro-electron diffraction (3D-ED). These developments have led to major advances in the characterisation of the atomic-scale structure of solid matter, from energy materials and green chemicals to glasses, proteins and pharmaceutical compounds.

The School was aimed at postgraduate students, early career researchers and newcomers to the field. It offered a series of lectures on the fundamental theory underpinning 4D-STEM and 3D-ED, together with historical background, software demonstrations and hands-on tutorials. The intensive program also included a live demonstration on MCEM's latest transmission electron microscope acquisition, the Thermo Fisher Scientific Spectra-j. A session was dedicated to presentations from industry scientists. There was also a lively poster session and a tour of MCEM facilities. The School was very fortunate to have twenty distinguished scientists from both overseas and Australia as its speakers. Amongst them were Ute Kolb (Johannes Gutenberg Universität Mainz) and Jian-Min Zuo (University of Illinois), past and present recipients of the Gjønnes Medal in Electron Crystallography, the highest distinction in the field. Over 70 delegates from 13 countries and 4 continents attended the School, with students and researchers from countries as far as Brazil, Belgium and China. This included a significant cohort from the X-ray crystallography community. Feedback from attendees was very positive, with appreciation shown not only for the quality of the program, but also for the opportunity to meet with the broad crystallography community. The organising committee is grateful for the generous support from the following sponsors: the IUCr, Microscopy Australia, the Society of Crystallographers in Australia and New Zealand (SCANZ), Rigaku, JEOL, Thermo Fisher Scientific, Dectris, ReadCrystal, Gatan Ametek and NanoMEGAS. The IUCr grants supported 13 PhD students and postdoctoral researchers, 4 of whom came from overseas (Belgium, Germany and China). More detail can be found on the ECS2023 website, <https://sites.google.com/monash.edu/ecs2023/>. The ECS2023 included presentations from many distinguished international scientists, here Prof. Lukáš Palatinus from the Czech Academy of Sciences.

Twelfth Belgian Crystallography Symposium BCS-12

Luc Van Meervelt

More than 70 participants took part in the Twelfth Belgian Crystallography Symposium

BCS-12, which was held in the Academy Palace in Brussels on 18 October 2023. The National Committee for Crystallography organizes this symposium at biennial intervals to promote contacts between Belgian scientists using diffraction and microscopy techniques for studies in the fields of chemistry and physics, material sciences, earth sciences and life sciences. Because one of the main objectives is to give young researchers an opportunity to present their results, the symposium program includes, in addition to plenary lectures, flash and poster presentations and short lectures by PhD students and postdocs.

During the opening lecture by Prof. Dorthe Ravensbæk (Aarhus University) a nice overview was given of how operando synchrotron X-ray diffraction and total scattering can be combined with pair distribution function (PDF) analysis to elucidate the structural evolution in a series of rechargeable battery electrode materials, which undergo varying degrees of disordering during charging or discharging. The morning session continued with nine flash presentations, including three from our sponsors.

Before lunch, a new microfluidics-based method for time-resolved cryo-EM sample preparation was presented by Prof. Rouslan Efremov (Free University Brussels). The method was developed for the study of molecular

machines and its application to the GroEL/ES chaperonin system required for assisted folding of many proteins was demonstrated.

During the lunch break, participants had time to visit the poster session and our sponsors.

In the afternoon Dr. Matthew Lightfoot (Cambridge Crystallographic Data Centre) highlighted the new possibilities with the Cambridge Structural Database, containing today more than 1.25 million structures, and its associated software. The knowledge derived from the structural data contained in the database has underpinned fundamental chemical discoveries and played a key role in designing new materials from drugs to pigments and beyond. The afternoon session ended with seven shorter lectures given by young researchers.

During the reception, two CCDC prizes were awarded to Marek Beliš (Ghent) and Thi Quintelier Matthias (Antwerp), together with IUCr Journals prize for Romy Poppe (Antwerp).

This BCS-12 meeting was sponsored by Bruker AXS, UCB, Rigaku, CGB-CBB, CCDC and IUCr Journals.

Crystallographic Society of Japan Annual Meeting and General Assembly

Kazuya Hasegawa and Hiroyoshi Matsumura

At Yamaguchi University, October 2023

<https://yamaguchi2023.crsj.jp>

The annual meeting and general assembly of CrSJ (CrSJ2023) were held at Yamaguchi University from October 27 to 29, 2023. In total, 273 crystallographers participated in the meeting, there were 160 oral and poster presentations covering all aspects of crystallography, three award lectures and five symposia. The young crystallographer's meeting was also held as one of the scientific sessions. Prior to the annual meeting, a satellite workshop on powder diffraction and total scattering was held on October 26.

The annual meeting started with the general symposium "Expanding Crystallography into Structural Science in Drug Discovery" (organizer: Prof. K. Iwasaki of Tsukuba University). More than half of the total attendees of the meeting participated in this symposium despite the diversity in the attendees' professions. Four more symposia, also determined by open proposals, were held in parallel on day 3: "Present Status and Future Prospects of Coherent X-Ray Diffraction Imaging" (organizer: Prof. M. Nakasako of Keio University); "Harmonic Interplay between Molecular Flexibilities and Crystal Rigidities" (organizer: Dr. H. Sugiyama of CROSS); "Protein Crystallographers Look at a New World Through Cryo-Electron Microscopy" (organizer: Dr. N. Muraki of Keio University); "Crystallography on New Material Synthesis and Process Development Using High Pressure" (organizer: Prof. T. Shimada of Hokkaido University).

At the CrSJ Awards Ceremony, the Nishikawa Award was presented to Prof. Tetsuya Ishikawa for his research "A new era in crystallography brought about by the realization of ultra-bright synchrotron radiation facilities: SPring-8, SACLA, and beyond", the Research Award was presented to Prof. Masahiro Fujihashi (Osaka Medical and Pharmaceutical University) for his research "Elucidation of enzyme mechanism as well as exploration and design of new enzymes, based on crystal structures", and the Young Crystallographer Award was presented to Prof. Yuki Takayama (Tohoku University) for his research "Development and Application of Multishot Coherent X-ray Diffraction Imaging." Five young scientists were honored with Student Presentation Awards based on their poster presentations on the first day: Mibuki Hayashi (University of Tsukuba) and Kazuki Hiraoka (Tohoku University) in the physics and mineralogy field, Shun Sumikawa (University of Hyogo) in the chemistry field and Keishiro Uda (Kyusyu University) and Midori Uenaka (Osaka University) in the biology field.

The Young Crystallographer's Committee organized a mini-symposium on the second day. Two invited young scientist speakers gave research presentations, and two graduate students presented their activities in the IUCr2023. After the presentations, 66 participants, including young researchers and graduate students over several research fields were separated into seven tables for group discussions. At each table, participants discussed and shared information on their research/campus life through crystallography.

A satellite workshop titled "Fundamentals and Practices of New Analytical Methods in Powder Diffraction and Total Scattering" was held in collaboration with Rigaku Corporation and had 35 participants. The purpose of the workshop was to provide a program for researchers who are interested in new analytical methods but are not confident in using them because they do not understand the fundamentals well or do not know how to apply them in practice because there are no experienced researchers in their institutions. Dr. Hideo Toraya, the developer of the Direct Derivation (DD) method, an innovative quantitative analysis method using powder diffraction, gave a lecture on the basics of the DD method. Dr. Masatsugu Yoshimoto presented the basics of the Pair Distribution Function (PDF) method and the Reverse Monte Carlo (RMC) method for total scattering pattern analysis. As a practical version of these analysis methods, Dr. Miki Kasari demonstrated the analysis of demo data using Rigaku's SmartLab Studio II software.

The chair of the organization committee was Prof. A. Nakatsuka (Yamaguchi University), and the program committee was chaired by Prof. K. Komatsu (University of Tokyo). The next annual meeting will be held from 8–10 October 2024 at Nagoya University in Aichi, Japan. The organization committee chair is Prof. L. Chavas (Nagoya University), and the program committee is chaired by Prof. S. Aoyagi (Nagoya City University).

The general symposium on the first day.

The recipients of the 2023 CrSJ Awards with the President of CrSJ. From left: Prof. A. Nakagawa (President), Prof. T. Ishikawa, Prof. M. Fujihashi and Prof. Y. Takayama.

The five poster Awardees at banquet. From left: M. Hayashi, M. Uenaka, S. Sumikawa, K. Hiraoka and K. Uda

Group photo at the Young Crystallographer's mini-symposium

CCDC news and updates

Author not stated in source

CSD Data Release (November 2023)

The fourth data release of 2023 adds 10,837 structures (11,411 new entries) to the Cambridge Structural Database (CSD). This takes the total size of the database to 1,254,560 structures (1,284,316 entries). This full release update all the existing entries, improvements to existing entries, and new entries. Knowledge bases like Mogul and Isostar have been updated.

Find out more about our releases and this latest data update [here](#).

If you are one of our thousands of contributors to the CSD don't forget to check out our social media channels in December to participate in [#CSDWrapped!](#)

November 2023 Update on Our Ongoing Investigations in to Structures Associated with a Pre-print on a Papermill in Crystallography

In April 2023 we provided an update to confirm 209 of the implicated structures had been retracted from the CSD following the retraction of 125 associated publications. These retractions left 783 implicated structures under investigation.

Working closely with publishers and our community, we are following COPE guidelines as our investigations progress. We continue to add editorial comments to entries to highlight information that may be relevant so users can select fit for purpose data. [Read more.](#)

Recent Blogs

Investigating Solid Form Stability: Understanding Hydrogen Bond Propensity in Mercury

Mercury allows you to view, analyse, and understand molecular structures and their properties. By exploring 3D structures, you can get a deeper understanding of the geometry of molecules, the way molecules pack together, and what voids and channels exist within a structure.

This blog explores Hydrogen Bond Propensity, a component within CSD-Materials that studies the hydrogen

bond network in a crystal structure, which was presented during the CCDC Virtual Workshop in October. Read the blog to learn more.

Unlocking Solid Form Innovation in CSD-Materials

CSD-Materials is a software suite that supports solid form development for crystal forms in the pharmaceutical and agrochemical industries. To enhance solid form reporting and research, the CSD Python API has been extended to cover more of the CSD-Materials suite, including parts of the Solvate Analyser, Hydrate Analyser and Aromatic Analyser components. Read the blog to learn more.

Improved CSD Torsion Data in GOLD

GOLD is the validated, configurable protein–ligand docking software for expert drug discovery, used for virtual screening through lead optimization. The torsion distributions sampled by GOLD during protein–ligand docking have been improved, including re-built and enhanced torsion distributions using the latest Cambridge Structural Database (CSD) and Mogul knowledge. Read the blog to learn more.

Upcoming Events

Visit our events page at [Events | CCDC](#) for more details on dates and topics.

Webinar: How Rapid Assessment of Molecular Geometries Can Help the Structure-Based Drug Designer

It is well recognized that the pre-organization of a ligand into a low-strain binding conformation is a valuable objective in drug design. Mogul software from CCDC enables a rapid assessment of the geometry of a 3D model. During this webinar, John Liebeschuetz, Computational Chemist at Astex Pharmaceuticals, will demonstrate recent work using Mogul, which validates the proposition that strained or unusual molecular geometries are seldom encountered in optimized drug molecules. When they do appear, they are often indicative of a crystallographic artifact. [Register here.](#)

If you would like to suggest topics for our workshops, webinars, and CSDU online training modules in 2024, please email us at hello@ccdc.cam.ac.uk.

Free Online Courses

Learn more about the Cambridge Structural Database (CSD), how to use CSD software and data to inform and advance your research, and how cheminformatics and structural chemistry can be applied to problems in the discovery and development of new molecules and materials.

The CSDU is a series of free on-demand training modules to learn at your convenience. Start anytime [here](#).

Follow us on Social Media

Want to learn more about CCDC events, blogs, case studies, and software updates? Follow us on [LinkedIn](#), [Facebook](#), and [Twitter](#).

Robert H. Blessing (1941–2023)

Tim Bohen

Bob Blessing alongside a C α trace of the T6 bovine insulin hexamer [Smith, Pangborn & Blessing (2005). *Acta Cryst. D*61, 1476–1482].

Robert (Bob) Harry Blessing, a chemistry professor at the University at Buffalo (UB), NY, USA, and an emeritus senior research scientist at Hauptman-Woodward Medical Research Institute (HWI), died on 23 October 2023 at the age of 82.

Considered a leader in the field of high-resolution experimental crystallography for electron density modeling, he collaborated on numerous research papers and spoke at many national and international conferences.

Born in Wilkes-Barre, PA, he graduated in 1962 from King's College in Wilkes-Barre. After completing a PhD in inorganic and physical chemistry at Ohio University in 1970, he held postdoctoral positions at the University of Lund, Sweden; the University of Pittsburgh; and UB. After four years as an Assistant Professor of Chemistry at Mercyhurst College in Erie, PA, he moved to Buffalo in 1978 to become a Research Scientist at HWI, formerly the Medical Foundation of Buffalo. There, he worked with emeritus researcher Dr G. David Smith on the crystal structure of insulin. He also developed algorithms and software for crystallographic data reduction and error analysis that are widely used in laboratories worldwide. He co-authored publications with Smith and 1985 Nobel Prize in Chemistry winner Herbert Hauptman.

In good voice. From left to right, Wilson Greatbatch, Herbert Hauptman, Bob Blessing and Lodovico Riva di Sanseverino sing at the 75th birthday celebration for Nobel laureates Herbert Hauptman and Jerome Karle in Buffalo in 1992. Photo contributed to the IUCr gallery by W. L. Duax.

Dr Blessing continued his work at HWI after he was appointed an Associate Professor of Chemistry at UB in 1991. He was promoted to Full Professor in 2001, and during that same year helped design the graduate studies program for the Department of Structural Biology in UB's Jacobs School of Medicine and Biomedical Sciences. He later served as the Department's Director of Graduate Studies and Chair.

On four occasions, he was a visiting professor in the crystallography laboratory at the Université Henri Poincaré, now Université de Lorraine, in Nancy, France, where he had a long collaboration with Claude Lecomte, Professor of Crystallography and Physics.

He was President of the Pittsburgh Diffraction Society and an active member of the American Crystallographic Association.

From left to right, Akihito Yamono, Tony Linden, Bob Blessing, Ludger Häming, Ton Spek, David Watkin and Larry Falvello, speakers at the Microsymposium on Absorption Corrections at the 18th IUCr Congress in Glasgow, UK, in 1999.

Dr Blessing is survived by his wife of 61 years, Barbara Ann; a daughter, Kimberly Blessing, a philosophy professor at Buffalo State University, and son-in-law, Tim Bohen; and two grandsons. Another daughter, Kirsten Blessing-Hanagan, a nurse in the neo-natal intensive care unit at the former Women and Children's Hospital, died in 2006.

For a list of papers by Dr Blessing appearing in IUCr journals [click here](#).

Anton Paar looks forward to its 60th anniversary celebrations

Barbara Pühr

Pioneer in Non-Ambient X-Ray Diffraction

When we at Anton Paar introduced the HTK 10 high-temperature chamber back in 1964, we made our mark in the history of non-ambient X-ray diffraction. The HTK 10 high-temperature chamber was capable of heating samples up to 1600 °C in order to study their structural changes by X-ray diffraction during heating.

Prior to this, non-ambient X-ray diffraction of various materials was mainly done with home-made equipment, but there was no real commercial heating chamber available on the market. This changed when we entered into this market 60 years ago. Since then, our knowledge and experience in X-ray diffraction, especially under non-ambient conditions, has steadily grown. This has led to our current broad portfolio of non-ambient X-ray diffraction attachments for studies between -190 °C and +2300 °C under different atmospheres (dry and humid) and pressures, as well as mechanical or electrical loads. Along with this complete portfolio, we also create customized solutions for our customers, something that helps make Anton Paar the market leader in non-ambient XRD.

60th Anniversary Celebration

In 2024, we will proudly celebrate our first milestone in the field of X-ray diffraction. As part of the anniversary celebrations, we're organizing the XRD excites: Non-Ambient XRD & Beyond Symposium, a scientific meeting with a strong focus on non-ambient X-ray diffraction in Graz, Austria, from July 9 to July 11, 2024. In addition, our Anton Paar subsidiaries will be organizing regional non-ambient X-ray diffraction workshops. Throughout the anniversary year, we have lots of things planned.

For more information, follow us on LinkedIn or click here:



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