INTERNATIONAL UNION OF CRYSTALLOGRAPHY

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IUCR JOURNALS NEWS

Unleash your research paper



In 2014 Kudos emailed 1966 IUCr authors inviting them to become part of a pioneering scheme to help them promote their work to a wider community. Of the original emails sent over 50% were opened. The industry standard across all publishing partners taking part in the programme was 17%. This open-rate figure suggests a healthy interest in the programme and supports an earlier study by Kudos which showed 84% of researchers think more could be done to increase the impact and visibility of their work.

Over the coming months we will see a number of new features and updates to the existing service which essentially guides authors through the process of publicizing their work by drafting lay summaries and sharing these summaries on social media, email, blogs and other services.

At the beginning of the process, authors are now able to claim their articles easily through ORCID; if the user already has an ORCID ID they will be able to enter it at the end of the Kudos registration process, enabling the accurate matching of relevant publications from the researcher's ORCID ID.

Further enhancements will see authors being able to opt in to monthly emails detailing recent Kudos activity around their paper; for example, authors will be able to follow how many times their Kudos page has been viewed and how many times their paper has been downloaded.

Of those who opened the original email, a smaller number went on to explain one or more of their publications in Kudos by writing short lay summaries. Our aim is to encourage more of our authors who are keen to promote their work to engage with the Kudos platform and write lay summaries about their work, focusing on the importance of the research to the wider community and some of the eventual applications of the work.

Evidence has shown those papers with lay summaries and supplementary information are discovered more frequently and enjoy significantly higher usage.

Once an author has written a lay summary, the next stage is to enrich the entry with supplementary material and then share within our community. The Kudos platform gives authors the tools to be able to manage this entire process within the researcher's usual workflow. The author is then able to measure the results of their efforts through carefully created reporting pages.

The website is also being improved to offer guidance on 'What can I do?' and 'Why should I do this?' to further encourage authors to actively participate in the promotion of their work.

An achievement bar to encourage authors to complete all the possible activities for their publication will be introduced and, along with the other enhancements mentioned in this article, a cleaner dashboard will make it easier for authors to take in data-at-a-glance and then drill down to the detail.

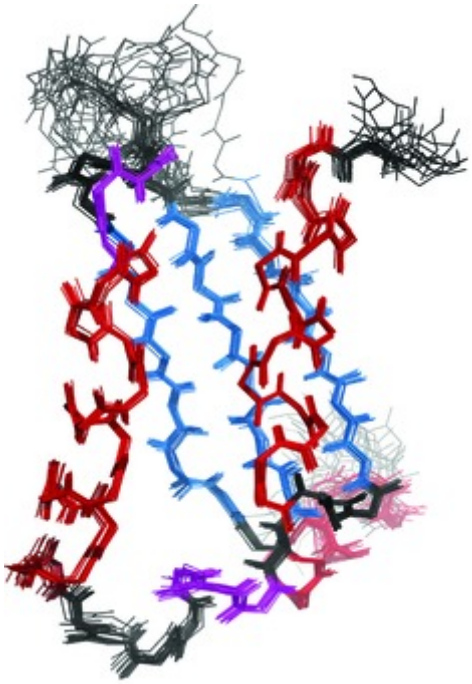
Over the course of 2015 more supporting material will be made available to authors *via* printed material distributed at conferences and rich media such as videos, podcasts and webinars to support authors in communicating their research to a wider, more interdisciplinary audience.

If you have any questions about Kudos please do not hesitate to get in touch.

Jonathan Agbenyega, IUCr Business Development Manager (ja@iucr.org)

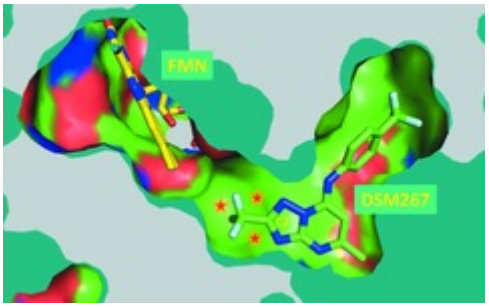
IUCR JOURNALS NEWS

Macromolecular crystallography and what it can contribute to antiparasite drug discovery



Solution-state NMR structure of BolA (PFE0790c) from *P. falciparum* [Buchko, G. W. *et al.* (2015). *Acta Cryst.* F**71**, 514-521].

The May 2015 issue of Acta Crystallographica Section F Structural Biology Communications (http://journals.iucr.org/f) is a dedicated special issue on the structural investigation of proteins associated with molecular parasitology, specifically research linked to protozoan pathogens. Parasitic protozoa threaten the lives of millions of human beings by causing a range of diseases including malaria, leishmaniasis, Chagas disease, toxoplasmosis and African sleeping sickness.



P. falciparum dihydro-orotate dehydrogenase complex with DSM267 and FMN [Hol, W. G. J. (2015). *Acta Cryst.* F**71**, 485-499].

Researchers have sought to understand the processes that allow pathogens to exist, to invade a host, to evade the immune response and to cause these debilitating and often fatal diseases. Structural biology, and in particular crystallography, complements such investigations. It can play a key role in drug

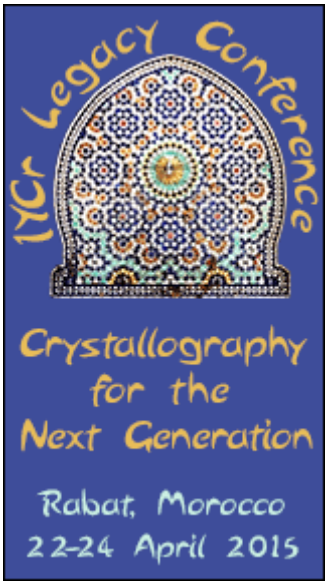
discovery by providing accurate chemical information to guide the assessment of drug targets and computational design projects, in the search for pharmaceutical compounds.

This special issue includes fundamental studies in molecular parasitology and also research directed toward protozoan drug target characterization, including both NMR and crystal structures. The articles include an overview and perspective from Wim Hol, an inspirational champion for the role of crystallography in drug discovery. There is also a short review from Inari Kursula on cytoskeletal proteins related to the infection process, a topic that may provide opportunities in future drug discovery work.

The publication of this special issue represents an exciting new departure for *Acta Crystallographica* Section F. The journal hopes to provide a natural home for new research in molecular parasitology, as well as welcoming contributions from the structural biology community as a whole.

IYCR 2014

Crystallography for the next generation: the legacy of IYCr



Hassan II Academy of Science and Technology, Rabat, Morocco
22-24 April 2015

Wednesday, 22 April
17:00-17:45 Opening Ceremony
17:45-18:15 Presentation of awards
18:15-19:00 Opening Lecture
19:00 Welcome cocktail

Thursday, 23 April
08:30-10:30 Session 1: Building capacity in crystallography
11:00-13:00 Session 2: Symmetry
14:30-16:30 Session 3: New opportunities in crystallography education
17:00-19:00 Session 4: Preparing for the future

Friday, 24 April
08:30-10:30 Session 5: Phosphates
11:00-15:45 Session 6: The IUCr 'Crystallography in Africa' initiative
15:45-17:00 Session 7: Outreach activities at large-scale facilities
17:30-19:00 Session 8: Initiatives and opportunities at the IUCr

The full programme for this conference, with details of all the speakers and links to the presentations, can be seen here.

IYCR 2014

Rigaku OpenLab Colombia, October 27–31, 2014



Organizing committee and Rigaku representatives of the Rigaku OpenLab Colombia. From left to right: Tomikatsu Kubo (Rigaku Corporation), Eric Reinheimer (Rigaku-USA), Graciela Diaz de Delgado and Miguel Delgado (ULA, Venezuela), José Antonio Henao (UIS, Colombia) and Akihiko Iwata (Rigaku-Latin America).

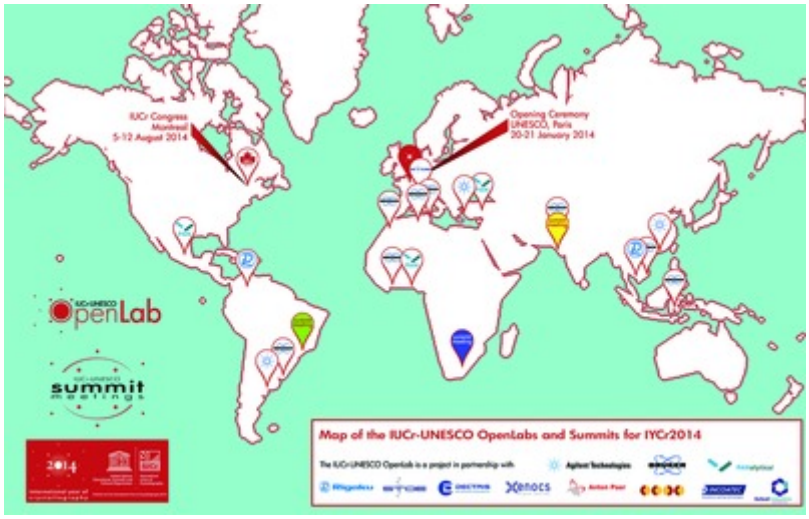


Students and instructors participating in the Rigaku OpenLab at UIS, Colombia.

The Rigaku OpenLab Colombia, dedicated to single-crystal diffraction, took place at the Guatiguará Campus of Universidad Industrial de Santander (UIS) in Bucaramanga, Colombia, on October 27-31, 2014. The Laboratorio de Rayos X of UIS hosted this course, which made use of the superb facilities of the laboratory, including the new dual-source Rigaku Single Crystal Diffractometer. The event was sponsored by the IUCr, Rigaku and the Vice-rectoría de Investigación y Extensión of UIS. Additional support was provided by Anditecnica and ICDD. Thirty four students and young scientists from Colombia, Venezuela, Bolivia and Costa Rica attended the lectures and practical sessions. The meeting was organized by Prof. José Antonio Henao (UIS, Colombia), Miguel Delgado and Graciela Díaz de Delgado (ULA, Venezuela) and Akihiko Iwata (Rigaku-Latin America). Eric Reinheimer (Rigaku-USA), Alexander Briceño (IVIC, Caracas, Venezuela) and Belkis Ramírez (ULA, Mérida, Venezuela), along with José Antonio

Henao, Miguel Delgado and Graciela Díaz de Delgado, delivered lectures related to symmetry, diffraction, data collection and reduction, structure determination and refinement, graphical representation and validation, among other topics. They were joined by Rodolfo Moreno Fuquen (Universidad del Valle, Cali, Colombia), Teresa González de Briceño (IVIC, Caracas, Venezuela), and Reinaldo Atencio and Julia Bruno-Colmenárez (IVIC-Zulia, Venezuela) for practical sessions. The OpenLab provided an excellent setting to strengthen the collaboration between Colombian and Venezuelan crystallographers and coincided with the celebration of Chemists' Day in Colombia on October 31. An event dedicated to powder diffraction is planned for 2015. The venue, Venezuela or Colombia, will be decided soon.

José Antonio Henao, Miguel Delgado and Graciela Díaz de Delgado, Organizers



Pakistan 30 Apr–8 May 2014
Argentina 5–10 May 2014
Morocco 26 May–20 Jun 2014
Ghana 9–12 Jun 2014
Cambodia 7–11 Jul 2014
Uruguay 23–31 Jul 2014
Indonesia 18–22 Aug 2014
Turkey 1–5 Sep 2014
OpenFactory 10–19 Sep 2014
Colombia 27–31 Oct 2014
Mexico 18–21 Nov 2014
Hong Kong 3–7 Dec 2014
Vietnam 8–12 Dec 2014
Turkey 2 19–22 Jan 2015
Algeria 9–14 May 2015
Tunisia 14–23 May 2015

This map shows the locations of the OpenLabs and OpenFactory that were organized by the IUCr and UNESCO in partnership with crystallographic instrumentation manufacturers during 2014 and early in 2015. These events provide the opportunity for local students and young professors in parts of the world where crystallography is as yet a poorly developed science to collect and interpret single-crystal or powder X-ray diffraction data in a university laboratory under expert guidance. More details and reports can be found in the IUCr Newsletter and at www.iycr2014.org/openlabs. The IUCr is keen to continue the OpenLab project and, with the help of the crystallographic community, transform it into a long-term sustainable initiative to promote capacity building, international cooperation and curriculum development.

IYCR 2014

Bruker OpenLab Vietnam, December 8–12, 2014



Students and instructors participating in the Bruker OpenLab in Vietnam.

The IUCr-UNESCO OpenLab Vietnam, organized in partnership with Bruker, was held at the Chemistry Dept. of the Vietnam National U., Ho Chi Minh City-U. of Science (VNUHCM-US) and the Center for Molecular and NanoArchitecture(MANAR), Ho Chi Minh City, in conjunction with IYCr2014 from December 8 to 12, 2014, with the purpose of promoting crystallographic teaching and research in South-East Asia.

The Opening Ceremony on Monday, December 8, was chaired by Nguyen Thi Thanh Mai, Dean of the Chemistry Department of the VNU-HCM-US, and a welcome speech was given by Vu Hai Quan, Vice-President of the VNU-HCM-US. After the opening session, Luc Van Meervelt started his intensive crystallography course on symmetry, X-ray diffraction, and single-crystal structure determination and refinement. The afternoons of the first three days were mainly dedicated to further exercises, supervised by Nguyen Bich Ngan (Hanoi), on point, plane and space groups, structure factor calculations, and a number of demonstrations such as Fourier transform and the use of the Cambridge Structural Database.

During the last two days, the participants visited the MANAR Center in smaller groups, where they could assist at a demonstration of crystal mounting and data collection and had the opportunity to collect diffraction data from their own crystals. In addition, data reduction, structure elucidation and refinement steps were introduced by Thanh-Ha Nguyen (Bruker AXS Singapore) and Bohari Bin Mohd (Malaysia) during hands-on training sessions.

During this five-day course, the lecturers aimed to introduce the main aspects of a single-crystal structure determination, andat the end each participant was able to solve and interpret independentlya crystal structure, as well as prepare CIF files for publication. In total 112 participants attended the course, including 12 international guests (from Thailand, Malaysia and Canada), 12 from outside Ho Chi Minh City and 84 from different institutes and universities in Ho Chi Minh City. Thanks to financial support from the IUCr, the MANAR Center and the VNU-HCM-US,the OpenLab Vietnam could be organized successfully, and the participants were very enthusiastic when they received their certificates during the Closing Ceremony.

Nguyen Tuyet Phuong (Ho Chi Minh City) and Luc Van Meervelt (Leuven)

IYCR 2014

PANalytical OpenLab Turkey, January 19-22, 2015





The OpenLab Turkey, organized within the frame of the International Year of Crystallography 2014 in collaboration with UNESCO and IUCr, was held in the campus of Bilkent U. at the National Nanotechnology Research Center (UNAM), January 19-22, 2015. The OpenLab logistics and organization were taken care of by the U. of Bilkent (Eda Yilmaz) and the Turkish Crystallographic Association (Süheyla Özbey) with the support of the IUCr, PANalytical BV, Atomika Teknik and UNAM.

The aim of the OpenLab was a broad introduction to the basics of crystallography, focusing on the theory and practice of powder diffraction, and on specific applications in the field of cultural heritage. Thanks to the powder diffractometer installed at UNAM, the attendees had the chance to participate in hands-on training with powder diffraction data collection and interpretation.

The scientific lectures during the four days of the OpenLab were delivered by Gilberto Artioli (U. di Padova, Italy). They included the nature of X-rays and their interaction with matter, basics of crystallography and diffraction, the experimental geometries for powder diffraction, data interpretation (including phase identification, quantitative phase analysis, available software, and databases) and an introduction to full profile refinement. Marco Sommariva (PANalytical) covered most of the applied aspects, such as the details of instrumental components, calibration and practical data collection.

A special effort was devoted during the OpenLab to present and operate freely available software, such as GSAS, and open-access databases, such as COD, in an attempt to direct the attendees towards independent crystallographic activities.

Extensive hands-on laboratories involving data collection on the available instrumentation and demonstrations on data treatment and analysis were followed with extreme interest. All the attendees showed a very active participation during sample preparation and basic measurements, as the participants also had the opportunity to measure their own samples and consult experienced crystallographers on specific cases. A few advanced applications were also shown, with the focus on materials science and application to cultural heritage. The session on cultural heritage was nicely complemented by lectures on archaeometry in Turkey (Ali Akın Akyol), on the use of nanoparticles for the conservation of paper material (Ayşen Yılmaz), and on the use of pair distribution function analysis (Bora Kalkan). The afternoon of the last day was devoted to a visit to the splendid Museum of Anatolian Civilizations in Ankara's old city centre.

The OpenLab Turkey event brought together over 30 participants from several countries (besides Turkey, attendees were from Albania, Egypt, Ethiopia, Iraq, Italy and Uzbekistan), selected on the basis of interest and country of origin from about 150 applications, the number of applications testifying the high interest for the event. All participants who successfully completed the lectures received a certificate of attendance. The participants were PhD students, researchers and young professionals from industry.

Very positive feedback was expressed by the participants during and at the end of the OpenLab event, both concerning the presentations and the practical sessions. The general impression is that the spirit and aims of IYCr2014 were conveyed, and that great interest has been aroused for future schools and workshops. Many participants repeatedly asked for future training and follow-ups.

On the final day the local committee met to discuss potential follow-ups, because not all the budget allowed for the event was actually spent. The proposal from the local committee was to organize a follow-up hopefully led by the Turkish Crystallographic Association. The idea is to combine training in basic powder diffraction and selected advanced applications, possibly transforming the event into a periodic school to beheld in different Turkish universities. There is a strong desire to consider the OpenLab as the triggering event for a regular and sustainable school for the Turkish (or even an enlarged) community. Periodic crystallographic training under the auspices and support of IUCr is envisaged. Prof. Artioli presented the recommendations to the IYCr2014 legacy ceremony in Rabat in April 2015

Gilberto Artioli (Padova) and Marco Sommariva (Almelo)

IYCR 2014

CRISTALLI@Parma: I wish I lived here







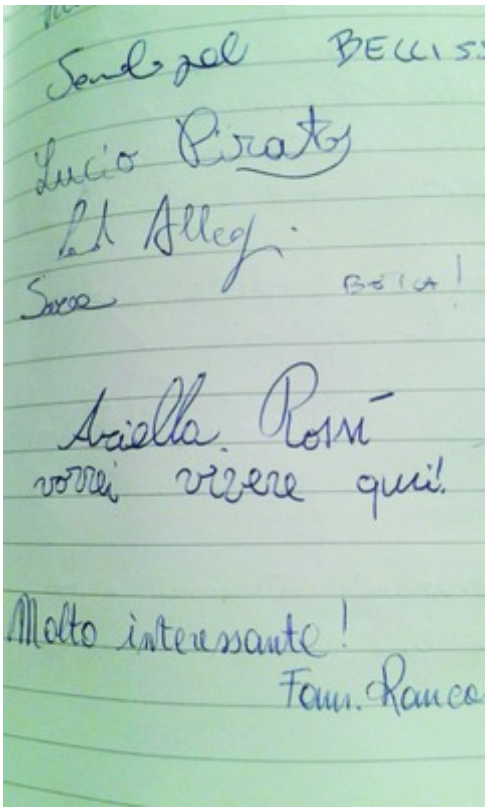
'The rocket', a silicon single crystal of 250 kg grown by the Czochralski method.



A giant model of NaCl made from glittering balls and sticks.



Participants enjoying a demonstration.



Extract from the visitors' book. Vorrei vivere qui: I wish I lived here!

Among the several initiatives carried out in Italy to celebrate IYCr, one of the most successful was the exhibition CRISTALLI!, promoted by the Italian Crystallographic Association. The exhibition started in Padua and was then reinvented in many other Italian cities with different flavours and views, like a wave travelling through the country. CRISTALLI!@Parma, organized by the University in collaboration with IMEM-CNR, had an amazing impact on the public, attracting 12,500 visitors in 7 weeks (http://cristalli.unipr.it/). The crowds attending the guided tours with experiments at the weekends were impressive, with everyone showing a real enthusiasm for crystals and ready to learn all the (crystalline) faces of cheese, ham, sugar, ice cream and medicines. The exhibition in fact was centred on showing the links between crystallography and the local excellence in food processing, pharmaceuticals and of course academic research.

All kinds of crystals were on display, from amazing sugar crystals weighing more than 0.5 kg to meteorites, minerals, shells and a silicon single crystal of 250 kg grown by the Czochralski method, immediately nicknamed 'the rocket'. A giant model of NaCl made from glittering balls and sticks was the kids' favourite. A special section of original artworks related to crystallography was organized in collaboration with the Archive of Modern Art of the U. of Parma. The exhibition booklet (www.mupeditore.it/saggistica/divulgazione_scientifica/cristalli.aspx) collected together simple explanations on crystallography related to daily life and recipes for growing one's own crystals, and was highly appreciated by visitors of all ages. The visitors' book was full of enthusiastic comments; the best was probably 'I wish I lived here' from Ariella.

Thanks to this precious IYCr legacy, the crystallographers in Parma, working in the Dept. of Chemistry and the Dept. of Physics and Earth Science, and at IMEM-CNR, are determined to build a network of contacts with schools to introduce subjects related to crystallography into the science lectures, and to continue to hold public lectures and open labs to bring the general public closer to the beauty of crystals. The training of high school teachers in the basics of crystallography is another extremely important activity promoted by the Italian Crystallographic Association through the realization of a completely original introductory book, in Italian, that is being distributed free all over Italy to high school teachers

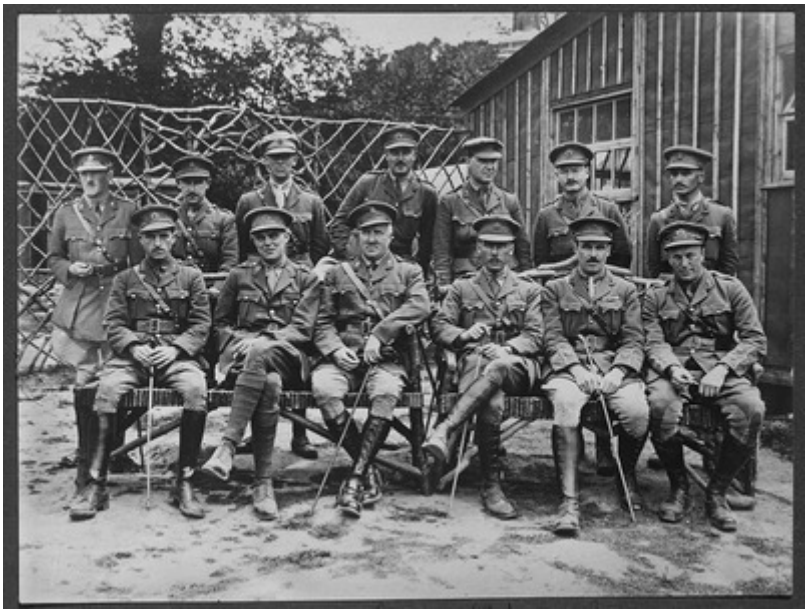
involved in projects between schools and universities. The book can be downloaded from the website of IYCr in Italy (www.iycr2014.it/contenuti/libro/49).

These are only two successful examples of how IYCr has really reached important targets in Italy, in raising public awareness of the importance of crystallography, reaching the youngest by exciting their imagination, and catching the interest of high school teachers, who are important in orienting young talents to scientific careers. We wish IYCr will be forever.

Alessia Bacchi

SPECIAL REPORT

How Lawrence Bragg shortened World War I



Lawrence Bragg (seated second from right) at General Headquarters in France in 1917 (photo: The Royal Institution, London, UK/Bridgeman Images).

As crystallographers we all know about W. L. Bragg and his role in founding X-ray crystallography. But how many know about his activities 100 years ago during World War I?

After his successes in solving several important crystal structures together with his father during 1913–1914, all research work ended with the outbreak of war. Bragg was commissioned as a Second Lieutenant in the Leicestershire Royal Horse Artillery in August 1914. One year later, he received a letter from the War Office instructing him to report to Colonel Walter Coote Hedley of the Royal Engineers. Hedley told him that the French had begun experiments to determine the location of the enemy guns by measurements based on sound waves (sound ranging), and proposed that he should go to France to head a unit to develop this method. He was assigned a young officer, Harold Robinson, a physicist who had worked with Rutherford in Manchester, and who was at the time serving in a coastal defence battery. They were sent to report to General Headquarters in France to meet Lieutenant Colonel Ewan Maclean Jack, who was in charge of the Field Survey sections. Later, these sections included Sound Ranging and Flash Spotting units (determination of the enemy gun positions by sighting their flashes).

Jack then sent them to the Vosges mountains to join up with a group of Sound Rangers. This section used a recording apparatus designed by Lucien Bull, a French physicist of Irish descent who was an expert on electrocardiography. This apparatus, built at the Institut Marey in Paris, consisted of a string galvanometer, where a fine string runs between the poles of a magnet. When an electrical current runs through the wire it is moved in the magnetic field, and the shadow of the wire is then recorded on a moving strip of photographic film. Bull’s apparatus had six strings attached to six microphones so that the time differences from receiving the gun report could be recorded.

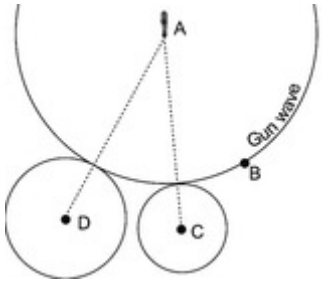
It was during this time that Bragg heard from Colonel Jack that his brother, Bob, had died of wounds during the 1915 Gallipoli campaign (the clever young physicist Henry Moseley, who had discovered the relationship between X-ray energy and atomic number, was also killed there in 1915). Bragg was sent to Paris to collect a recording set and he set up the first sound-ranging station at Kemmel Hill just south of Ypres. Six microphones were placed about one mile behind the front with the recorder in a small village called La Clytte. It was here in November 1915 that he heard by telegram that he and his father had

been jointly awarded the Nobel Prize in Physics. Bragg recalled that the friendly priest, in whose house they were billeted, brought up a bottle of Lachrimae Christi from the cellar to celebrate the occasion.

The early sound-ranging experiments were disappointing and their results of little value. The problem was with the microphones, which were unsuitable to pick up the gun sounds. When a high-velocity gun fires a shell with an initial velocity greater than that of sound, the shell creates a wake or 'shell wave', which is heard as a loud crack. This crack is far more intense than the low-toned 'wuff' which is the true gun report, and on which the sound-ranging measurements had to be made. Their microphones, of a type used for long-distance telephony, were far more sensitive to the shell wave than to the gun report, which tended to be completely obscured by the loud crack. They were also sensitive to rifle fire, traffic noises, general battle sounds, swearing by the troops and dogs barking.

The problem was solved a year later, when Bragg was sitting on the privy in a hut which had an opening to the outside: when a nearby British gun fired, his bottom was lifted off the seat, even though he had heard nothing. He realized that the gun wave created a pressure spike and that this could be used to detect it. Bragg teamed up then with Corporal William Tucker, who had studied physics in London. Tucker knew that the pressure change could be detected by recording the change in electrical resistance of a hot platinum wire: the cooling puff of air caused by the pressure change increases its resistance.

They then rigged up a crude microphone (later called the Tucker microphone) based on this idea using an ammunitions box inside which the wire was stretched across and which had a small opening to allow air to enter. They immediately saw that the wire reacted to the gun report and ignored the shell wave.



The method of location was both ingenious and simple (see the figure), typical of Bragg's approach. The gun at A fires and creates a gun wave that eventually arrives at microphone B. After this it reaches C and then D. Now, by knowing the velocity of sound under the air conditions of the time (one way was to carry out actual measurements with known cannon fire), circles can be drawn around C and D corresponding to the time differences from B. This allows the gun wave circle through B to be constructed, and then lines drawn back from C and D locate the gun.

The system was finally deployed in earnest at the front using about 40 miles of low-resistance insulated wire between the microphones, although they were exposed to destruction by enemy fire but more importantly to pilfering, especially by Australian troops!

So successful was sound ranging using this method that it seriously affected the ability of the German guns to operate. Perhaps the most spectacular success was had at the Vimy Ridge where German guns were firing at Canadian troops from the shelter of woods. Looking back at Bragg's sound-ranging work, we can see that he and his team had played a significant part in shortening the war and bringing it to an end in 1918. Interestingly, the same method was used in World War II. However, in the interwar years, the system had been 'improved' by adding several technical advances. Much to Bragg's delight, it was found that this actually degraded the performance of the simple Tucker system and in the end they had to revert to his earlier design.

More details can be found at http://rsnr.royalsocietypublishing.org/content/59/3/273.full and in the book Crystal Clear: the Autobiographies of Sir Lawrence and Lady Bragg by Mike Glazer and Patience Thomson, to be published this summer by Oxford University Press.

Mike Glazer

SPECIAL REPORT

'Seeing the light'



The Cambridge Backs behind St John's College. Photo courtesy of Dr John Leake.

Just occasionally someone has an idea so profound that it changes the world and how we see it. One such idea reported in the very first science paper written by a 22-year-old graduate student has turned out to be one of the most influential.

G. H. Hardy wrote 'The mathematician's patterns, like the painter's or the poet's, must be beautiful; the ideas, like the colours or the words, must fit together in a harmonious way. Beauty is the first test'. In the afterglow of IYCr2014, it is worth celebrating Bragg's equation, which earned Lawrence Bragg and his father, whose X-ray spectrometer powered its exploitation, the Nobel Prize in Physics 100 years ago. It is a testament to the beauty and power of this discovery that he is still the youngest person ever to receive a Nobel Prize for science.

Lawrence Bragg had a remarkable mind. He had entered the University of Adelaide at 15 to study mathematics, moving to England at 18 when his father transferred to Leeds, and entered Trinity College Cambridge to again read mathematics. After a year at Trinity, upon his father's advice, he changed to physics (Natural Science). Yet as a new research student in the Cavendish Laboratory, he was unhappy. In his own words: 'It was a sad place at the time. There were too many young researchers ... too few ideas for them to work on, too little money, and too little apparatus.'

Despite this malaise, three key aspects converged within the mind of that young postgraduate student as he walked behind St John's College, Cambridge, one evening. It is perhaps interesting to look back at the events that culminated in that Damascene moment. It had all started a few months before when he joined his parents in Cloughton, on the Yorkshire coast, in the summer of 1912.

His father had just received a letter from his Norwegian friend Veygard, who described a lecture given by von Laue in Würzburg (where Veygard was working with Röntgen) in which he described how, on passing a beam of X-rays through a crystal, he obtained a series of spots in a pattern having the same symmetry as the crystal on a photographic plate. Laue had claimed this was due to 'diffraction' from waves. This set the Braggs off on their adventures. As his father believed X-rays were not waves but more like corpuscles or 'bullets', he and his father set about trying to explain the photograph in other ways.

Upon returning to Trinity, three things came together in Lawrence’s thoughts. First, J. J. Thomson had suggested in his lectures that X-rays were waves generated by the sudden stopping of electrons by a target. Secondly, C. T. R. Wilson, whose optics lectures he had attended, had shown white light could be considered as a continuous range of wavelengths (or pulses, as he called them). Finally, upon attending a Trinity College Science Society meeting he heard a paper suggesting that atoms in crystals could be thought of rather like spheres arranged in parallel sheets.

'I can remember the exact spot in the Backs where the idea suddenly leapt into my mind that Laue's spots were due to the reflection of X-ray pulses by sheets of atoms in the crystal' (unpublished memoirs). However, he soon hit upon a problem: his new theory didn’t match up with Laue's spot pattern obtained on cubic zinc blende. His mind went back to the Science Society meeting, where the presenter had explained that cubic crystals need not only have spheres located at the corners but also on the faces of the cubes. With this last piece of information everything clicked into place. In his famous paper to the Cambridge Philosophical Society in 1912 he famously proposed that Laue's results arose from the reflection of a continuous range of X-ray wavelengths (unlike the 6 or 7 distinct wavelengths assumed by Laue) by planes of atoms within the crystal. This interpretation yielded Bragg's law of X-ray diffraction: $n\lambda = 2d\sin\theta$, where θ is the angle of incidence of X-rays of wavelength λ, d is the separation of the reflecting planes and n is an integer.

Armed with this equation, and his father's X-ray spectrometer, they worked furiously in 1913 and 1914, going back in the evenings to the deserted university to obtain more and more measurements. He said it was like 'discovering a goldfield with the nuggets just lying there to be picked up. One could not resist the temptation to pick up more and more, without a rest'.

It is interesting to note that not until after the First World War did the world really wake up with shock and exhilaration to these papers; shock, because Bragg had incontrovertibly established, contrary to what all chemists thought at the time, that there was no molecule of sodium chloride inside rock salt - simply an extended alternation of sodium and chloride ions. Henry Armstrong, a former president of the Chemical Society of London, wrote in Nature in 1927 that the 'chess-board pattern' of atoms in sodium chloride was 'repugnant to common sense' and 'absurd to the nth degree'. Others were exhilarated because the structure of diamond confirmed the tetrahedral coordination of carbon as envisaged by J. H. van't Hoff and others some 40 years earlier.

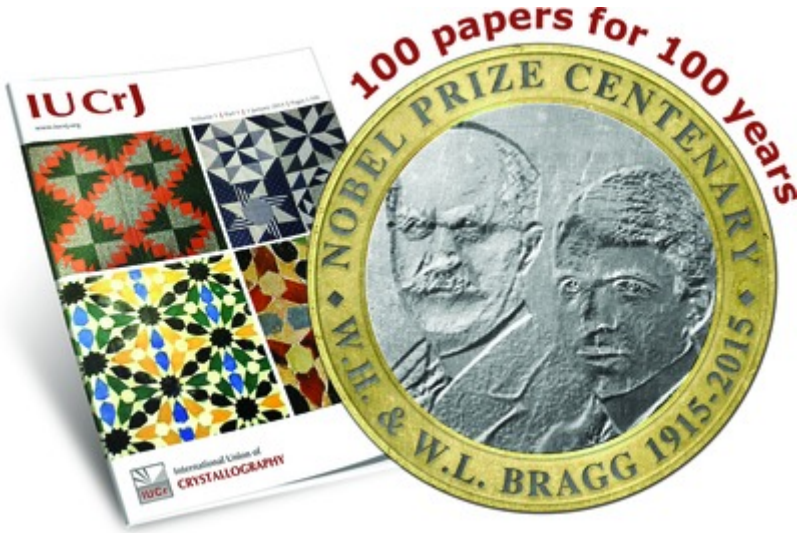
Moseley, who would not have completed his ground-breaking work without one of William Bragg's spectrometers, wrote to his mother after giving a lecture at which William Bragg was present: 'I was talking chiefly about the new German experiments of passing X-rays through crystals. … After much hard work Darwin and I found out the real meaning of the experiment, and of this I gave the first publication on Friday. I know privately however that Bragg and his son had worked out an explanation a few days before us, and their explanation although approached from a different point of view turns out to be really the same as ours. We are therefore leaving the subject to them. The subject is very important, and there will probably be an enormous amount of work done on it in the next few years'. Of course the subject hasn't been left to them and has maintained our interest over the last 100 years. Indeed, X-ray crystallography has transformed the very fabric of mineralogy, chemistry, metallurgy and biology, with vast databases holding X-ray-determined structural information on millions of compounds, inorganic, organic and biological, and contributed to more than two dozen Nobel Prizes.

So next time you see a student stopped in their tracks, leave them to their thoughts ... they might just have thought of something really beautiful.

Philip J. Withers and Sir John Meurig Thomas

IUCR JOURNALS NEWS

100 years, 100 papers



To commemorate 100 years since the award of the Nobel Prize to the Braggs for the first use of X-rays to determine a crystal structure, IUCrJ aims to publish 100 papers in 2015.

The first 100 articles submitted to IUCrJ using the voucher code below, and accepted for publication following peer review, will be published as platinum open access (*i.e.* there will be no charge for open-access publication).

Voucher code: **dis-63gwUYye619PkvwixPj**

FEATURE ARTICLE

Crystallography in Norway





35 men and women from Norway are listed in the first edition of the World Directory of Crystallographers from 1957. That is a large number coming from a population of about 4 million at that time. The number listed increased to 76 in 1971 and has since decreased to 43 today. In 1957 some working with crystallography were not listed, and in the list to day several have retired. Furthermore, those listed in 1957 were mainly determining crystal structures from X-ray diffraction data. Today, those listed have a wider interest in crystallography.

I will, in this article, concentrate on the work done by Norwegians active in determining crystal structures – mostly the pioneers active in Norway up to about 1990. Two Norwegian crystallographers educated in Norway are included (Zachariasen and Hope), but they went to the USA where they worked for the rest of their lives, but kept contact with colleagues in Norway.

The dominating activity has been in Oslo. I have received information about the history of crystallography in other citiesin Norway from E. Sletten (Bergen, Norway), T. Dahl (Tromsø, Norway) and F. Mo (Trondheim, Norway). I am grateful for their cooperation and contributions.

Classical crystallography



Peter Waage

The study of the external shape of crystals, classical crystallography, started in Norway at the Royal Norwegian Mining School at Kongsberg in the 18th century with the Danish Professor M. T. Brünnich (1737-1827), director of the silver mines. He published a book about Norwegian minerals in 1777. P.

Waage and H. Mohn wrote the first Norwegian textbook on crystal shapes in 1859. (Waage is known for his contribution to the law of mass action, also called Guldberg and Waage's law.)

Crystallography at the University of Oslo

Department of Physics



Lars Vegard

L. Vegard (1880-1963) was the pioneer in X-ray crystallography in Norway. He graduated with a master's degree from the Royal Frederik's U. (Oslo), then called Kristiania, the only university in Norway up to 1946. He worked as an assistant to K. Birkeland (1867-1917) on research connected with the Aurora Borealis. The spectrum of Northern Light became the main field of interest in his career, but he was also active in X-ray crystallography.



Central campus of the University of Oslo, where today only the faculty of law is located. Licensed under CC BY-SA 3.0 via Wikimedia Commons - http://commons.wikimedia.org/wiki/File:Universitetet_i_Oslo_sentrum.jpg#/media/File:Universitetet_i_Oslo_sentrum.jpg

In 1909 Vegard worked in the laboratory of W. Bragg (Leeds) and in 1911-1912 in the laboratory of W. Wien (Würzburg). In early June 1912 he attended a presentation by M. von Laue, who showed the sensational diffraction pictures that had been taken in Munich a few months earlier. Vegard wrote to Bragg and told him about 'certain new curious properties of X-rays' and included a copy of some of the pictures, inspiring the work by L. Bragg and his father W. Bragg.

Following his return to Norway, L. Vegard received his Dr. Philos. degree in 1913 with a dissertation on light emitted from canal rays. In 1918 he became the successor to Birkeland as full professor.

Vegard built his first X-ray diffractometer in 1914 and determined the crystal structure of silver. He started work on mixed crystals; von Laue mentioned this work in his Nobel Prize acceptance address in 1915. Vegard and about fifty of his graduate students worked in X-ray crystallography for thirty years. In

1920 Vegard published what has been called Vegard's law, 'The lattice constants of a mixed crystal vary linearly with the composition'. The law is still quoted in the literature.

Vegard also did pioneering low-temperature (liquid hydrogen) work, resulting in the determination of the crystal structures of a number of small-molecule substances that are gases at room temperature. Noteworthy among these are the structures of N_2 and O_2.

When a nuclear reactor was built at Kjeller just outside Oslo in the early 1950s, work was started to use neutrons for determining crystal structures. A. F. Andresen (1923-1991) began as a graduate student in physics at Kjeller and continued to work there the rest of his life. He used neutron diffraction to study the structure of magnetic compounds and was a pioneer in the study of the structures and properties of metal hydrides as potential materials for energy storage. For 15 years Andresen was a member of the Commission on Neutron Diffraction of the IUCr, three years as its Chairman. Another active researcher at Kjeller was the physicist Tormod Riste (1925-1996) working in solid-state physics.

None of Vegard's students continued working in crystallography. J. Gjønnes (1931-), who is the best-known Norwegian physicist in crystallography, belongs to a different tradition, from C. Finbak, H. Viervoll and N. Norman with connection to O. Hassel's group in physical chemistry (see below). In the early 1960s Gjønnes spent some time in J. Cowley's group in Melbourne. After returning to the U. of Oslo in 1965, Gjønnes established a group in electron microscopy and electron diffraction crystallography at the Dept. of Physics at the U. of Oslo. The experimental work covered a wide field of materials science. Theoretical studies included various aspects of dynamical electron diffraction: on symmetry, notably the so-called G-M (Gjønnes-Moodie) lines; methods for precise determination of structure factors, as well as the effects of dynamical diffraction on diffuse scattering and spectroscopic signals in electron microscopy. In recent years he has been engaged in developing the novel technique of precession electron diffraction as a practical tool for solving crystal structures. In 2008 his contributions to electron diffraction crystallography were recognized by a medal (named after him), of which he was the first recipient. Groups in Trondheim as well as in Oslo have continued the work in electron microscopy and electron crystallography. Gjønnes has been a member of the IUCr Commission on electron diffraction.

Mineralogy



Victor Moritz Goldschmidt

V. M. Goldschmidt (1888-1947) is the giant in Norwegian crystallography. He is the father of modern geochemistry and was proposed several times for the Nobel Prize in chemistry.

Goldschmidt was born in Zürich, but came to Norway at the age of thirteen. He learned classical crystallography from T. Hiortdahl (1839-1925) working in his private laboratory at Kristiania U. in 1906. Goldschmidt compared Hiortdahl to P. von Groth (1843-1927) and gave him credit for his systematic experimental work in chemical crystallography from 1862 to 1885, resulting in the introduction of the concept of partial isomorphism. Goldschmidt received his Dr. Philos. degree in 1911 when only 23 years of age. His dissertation was a monumental work on the geology of the Oslo region by showing that Gibbs' phase rule also applied in nature. Goldschmidt was appointed professor of crystallography, mineralogy and petrography and head of the Inst. of Mineralogy in 1914.



V. M. Goldschmidt (right) teaching E. Q. Berner classical crystallography in 1915. Berner (1893-1983) later became professor of organic chemistry at UiO in 1934.

In 1920 the institute (and museum) moved to a new building at Tøyen on the outskirts of the city. There he formed a research group and started systematic studies of minerals, determining the composition from X-ray spectroscopy and the crystal structure by X-ray crystallography, using equipment built at the museum. The results were published from 1923 to 1938 in nine volumes on 'The geochemical laws of distribution of the elements' (German). A mineral is not a pure chemical compound, and Goldschmidt found that the main ions in a mineral could be substituted with other ions of the same size and charge. He determined the ionic radii (the Goldschmidt radii) that explained the lanthanide contraction.

Goldschmidt also inspired his students to go into X-ray crystallography. The best known of his students who founded their own schools in X-ray crystallography are W. H. Zachariasen (1906-1979), O. Hassel (1897-1981) and H. Haraldsen (1906-2001).

W. (Willie) Zachariasen grew up close to the Langesund fiord, known for its islands with many rare minerals. When he finished high school in 1923 he started his studies at the University and was selected as a member of Goldschmidt's research group. He received his Dr. Philos. degree in 1928 on crystal structure determinations of oxides – the youngest person to obtain a doctor's degree in Norway (only 22). He was a master of interpreting powder diagrams. After a year as a postdoctoral fellow with L. Bragg (Manchester), he joined the faculty of physics at the U. of Chicago. There he stayed for the rest of his life. He contributed significantly to the theory of X-ray diffraction, as reflected in his book, *The Theory of X-Ray Diffraction in Crystals*. Zachariasen is known for his work on the determination of the structures of many of the radioactive elements and compounds produced during the Manhattan project from 1940 and onwards.

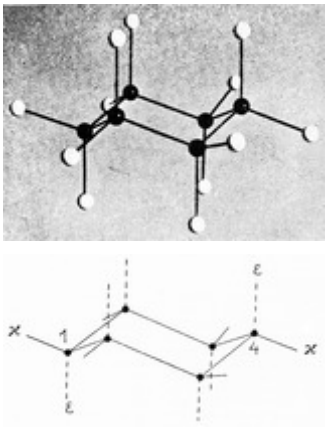
The best known from Goldschmidt's group at Tøyen that continued with mineralogy and geology is T. Barth (1899-1971). He determined the structure of several inorganic compounds. From 1929-1936 he worked as a crystallographer in the Geophysical Laboratory in Washington. He succeeded Goldschmidt in 1937 and was head of the Museum of Geology and Mineralogy from 1949 to 1958.

Physical chemistry (structural chemistry)



Odd Hassel (to the left) with a group of students going on an excursion in the summer of 1934.
O. Hassel (1897-1981) started his studies at the University in 1915 with Goldschmidt as his mentor. He wrote his Master's thesis on rates of certain chemical reactions, with H. Goldschmidt (1857-1937), the father of Victor, as his advisor. He went abroad to study at the K. Wilhelm Inst. in Berlin-Dahlem, where he learned X-ray diffraction, and obtained his Doctor's degree in 1924 at the Friedrich Wilhelms U. His closest advisor/colleague was H. Mark (1895-1992), later known as the father of polymer science.

In 1925 Hassel returned to the Laboratory of Chemistry in Oslo where new X-ray equipment awaited him. When Goldschmidt accepted a professorship in Göttingen, Hassel took over the laboratory at Tøyen, where he determined the crystal structure of several inorganic compounds, including graphite and the closely related boron nitride. In 1934 he published the book Kristallchemie in German that was translated into English and Russian. He became a full professor of physical chemistry the same year, the first such professorship in Norway.



Illustrations from Odd Hassel's paper 'The Cyclohexane Problem' [*Tidsskr. Kjemi. Borgv. Metallurgi*, Bd 30, nr 5A, 18, Jun 1970] describing the stereochemistry of cyclohexane based upon his electron diffraction studies, for which he was awarded the Nobel prize in chemistry in 1969.
Hassel became interested in the structures of organic compounds, in particular cyclohexane and its derivatives, but the structures were too complex to be solved by X-ray crystallography in the 1930s. He measured dipole moments that could tell something about the symmetry of molecules and turned to electron diffraction as a method for determining the structure of organic molecules in the gas phase. He established a research group in physics and chemistry. The most prominent members were C. Finbak (1904-1954) and H. Viervoll (1914-2005). Finbak invented the rotating sector and was central in the construction of the first electron diffraction instrument in Oslo. He also used X-ray methods to study the rotation of ions in solids and the structure of liquids. Viervoll refined the computational methods for

electron diffraction of gases and built the first electronic computer in Norway. The group in Oslo became a leader in the field of gas electron diffraction.

In the early 1940s Hassel and coworkers published the structures of cyclohexane and cyclohexane derivatives that earned Hassel the Nobel Prize in chemistry in 1969, shared with D. Barton (1918-1998).

In the 1950s, Hassel's group broke up into one group for electron diffraction studies of gases, one for X-ray diffraction of crystalline compounds and one on spectroscopy (IR, UV and Raman).

In his last ten years of active research, together with his students, Hassel began to study charge-transfer compounds. The first structures, compounds of dioxane and bromine and of dioxane and $HgCl_2$, were determined by J. Hvoslef (1926-1986), and compounds of aliphatic amines and halogens were determined by K. Olaf Strømme (1929-). These studies showed that the structures of the charge-transfer compounds are quite different from the structures proposed earlier by the spectroscopist R. Mulliken (1896-1986). Hvoslef received his Dr. Philos. degree in 1972 and went on to use neutron diffraction at Kjeller to determine H-atom positions. Strømme obtained his degree on structural aspects of molecular disorder in 1974. Both worked as lecturers at the department for the rest of their professional lives.

Due to the low melting points of some of the charge-transfer compounds, the X-ray diffraction group in Oslo had to develop methods for collecting data at low temperatures, first using a Weissenberg camera, and later manual and automatic diffractometers.

The best known of Hassel's students working with X-ray crystallography are S. Furberg, C. Rømming, B. Fjærtoft Pedersen, T. Dahl and H. Hope.



Sven Furberg showing a student how the diffractometer works.

S. Furberg (1920-1983) is famous for the determination of the structure of cytidine in 1948. He also proposed models for DNA that contributed to the Watson and Crick model in 1953. His best-known students are A. Hordvik (see below) and A. Mostad (1929-), who determined the crystal structures of several organic molecules of biological interest including L-dopa. Mostad worked together with Christian Rømming for many years, and has written a series of popular articles in Norwegian on elements and simple chemicals.

C. Rømming (1928-) introduced new equipment and new methods for handling crystallographic data in Oslo from Hassel's time in the 1950s to long into his own retirement years.

E. Wang Lund (1919-1979), the first to use Fourier methods in Norway, learned about them in Gunnar Hägg's laboratory in Uppsala in 1948. After 1960 he concentrated on teaching and writing textbooks.



Berit Pedersen, Henk Schenk, Peter Paufler, Yvonne Mascarenhas at the 1990 IUCr Congress and General Assembly in Bordeaux, France.

B. Fjærtoft Pedersen (1933-) worked at the Central Inst. of Industrial Research and became the first woman crystallographer in Norway when she was awarded the Dr. Philos. degree for the elucidation of the structure of perhydrates in 1969. She returned to the Dept. of Pharmacy at the university in 1972 where she concentrated on determining the crystal structures of drugs and imaging compounds.



Håkon Hope

H. Hope (1930-), after receiving his Cand. Real. degree in 1958, stayed on as an assistant to O. Hassel, working on charge-transfer compounds. In 1961 he received a Fulbright fellowship and spent two years at UCLA with J. D. McCullough and K. N. Trueblood. In 1965 he accepted a professorship at the Dept. of Chemistry, U. of California, Davis. Hope advanced the accuracy of diffractometry to optimize the information obtainable from diffraction data. He used the anomalous scattering from oxygen to determine the absolute configurations of molecules, and pursued the accurate measurement of electron densities and the determination of molecular geometries free of valence electron distortions. During a visit to the U. of Oslo, he developed equipment and techniques that facilitated diffraction measurements at liquid nitrogen temperatures.

In Davis in 1972, low-temperature measurements became the standard mode of operation for everyday structure determination. An important mission was to advance X-ray crystallography as a rapid, first-choice analytical method. Before area detectors, same-day structure service had become commonplace in Davis. To help study extremely reactive compounds, Hope developed methods that allowed simple, open-air manipulation of reactive or low-melting crystals. He modified these methods for use with biocrystals, first demonstrating their utility with small proteins, and then by showing that low-temperature diffraction data could be obtained from crystals of ribosome particles. The winners of the 2009 Nobel Prize in Chemistry used the methods with advantage. Hope was a coeditor of *Acta Crystallographica* (1984-1993) and received an honorary degree at the U. of Oslo in 1994.

T. Dahl (1938-) was Hassel's last graduate student. He graduated in 1963 and after some years as Hassel's research assistant he went to the U. of Tromsø, where he was awarded the Dr. Philos. degree in 1976 for his structure determinations of addition compounds between hexafluorobenzene and methylated benzenes. His later work comprises structure determinations of various addition compounds and substituted adeninium compounds.

Inorganic chemistry (solid-state chemistry)

H. Haraldsen established a research tradition that is still active at the Dept. of Chemistry at the U. of Oslo. Haraldsen worked as an assistant to Goldschmidt and wrote his Master's thesis on an X-ray and thermal analysis of two minerals. In 1932 he received his Doctor's degree with W. Biltz (1877-1943) in Göttingen on the thermal analysis of three phosphides. He studied magnetochemistry in Danzig with W. Klemm (1896-1985). Klemm was interested in transition metal chalcognides, an interest that occupied Haraldsen for the rest of his life. (The term chalcognides for the elements in group 16 in the periodic table was coined in Klemm's group in Danzig.)

In 1936 Haraldsen returned to Oslo where he became a full professor, succeeding the radiochemist E. Gleditsch (1879-1968). He established the second X-ray diffraction laboratory at the Dept. of Chemistry. Haraldsen was head of the division of general and inorganic chemistry, which is a section in the department. He built up laboratories for the high-temperature synthesis of chalcogenides, did phase analysis of *d*-metal/chalcogenide systems, determined the structures of the phases discovered by X-ray diffraction, and measured their magnetic, electric and thermal properties. He and his co-workers, F. Grønvold (1924-) and A. Kjekshus (1932-), guided graduate students who determined a number of crystal structures by X-ray diffraction. Some of these students are still active in the department, now called material or nano sciences. The current leaders are H. Fjellvåg (1954-) and S. Stølen (1960-).

The successor to Haraldsen in 1976 was P. Kofstad (1929-1997) who is known for his work on the defect structures of transition metal oxides. He wrote textbooks and studied high-temperature corrosion and the structure of non-stoichometric compounds. This work is carried forward today by T. Norby(1955-).

Department of Chemistry, UiO today

In 2003 the research in the department was reorganized into two sections: Section A, *Life sciences chemistry*, and Section B, *Functional materials chemistry*. Both sections have X-ray diffraction laboratories. The laboratory in A studies single crystals and in B mainly powders.



Carl Henrik Gørbitz

Early attempts by C. Henrik Gørbitz (1961-) to start protein crystallography were not very successful. The activity was expanded when U. Krengel (1964-) joined section A in 2004. She took her PhD in Heidelberg in the group of K. Holmes at the Max-Planck-Inst. for Medical Research (1988-1991; supervisor: E. Pai). As a postdoc she worked in Toronto with Pai and in Groningen with B. Dijkstra. In 1997, Krengel moved to Chalmers U. of Technology in Gothenburg where she established her own group focusing on protein-carbohydrate interactions. In Oslo she has set up an entire production line from gene cloning to final refined structure. Structures solved include those of anti-tumour antibodies, bacterial toxins, mushroom lectins and chorismate mutases, and work is being extended to include membrane proteins and large glycoproteins such as the human mucins. All projects involve international collaborations, with scientists from Sweden, Switzerland (ETH), Cuba and the USA.

Crystallography at the University of Bergen

The U. of Bergen was established in 1946. O. Foss (1918-2007) introduced X-ray crystallography when he was appointed professor of chemistry in 1955. He had used the method in his pioneering work on establishing the un-branched structure of the sulphur chains in polythionates. Later his research also encompassed the chemistry and structure of divalent selenium and tellurium compounds, and he was the first to study the structures of tellurium(II) complexes with ligands like thiourea, thiocyanates etc.

During the first two decades after Foss' arrival in Bergen the group of structural chemists grew steadily, the majority of its members working mainly on compounds of sulphur, selenium and tellurium. A. Hordvik (1928-1995) and his students were scientifically very productive in this group, especially in the study of cyclic dithioles and thiathiophthenes and thiathiophthene analogues. In 1974 Hordvik left Bergen to establish new activity at the U. of Tromsø (see below). S. Husebye (1933-), after obtaining his PhD from Tulane U., returned to Bergen where he studied a variety of chalcogen compounds, with special attention on highly coordinated tellurium(IV) complexes. K. Marøy (1930-) collaborated extensively with Olav Foss for a long period, and in later years worked on salts of selenates and tellurates together with S. Hauge (1932-). K. Maartmann-Moe (1928-) joined the group in 1965 and became the manager of the X-ray laboratory equipment when the first single-crystal diffractometer was purchased in 1968, a responsibility he held until his retirement in 1995.

The scope of structural chemistry in Bergen was gradually broadened to include work on transition metal complexes. In 1967 E. Sletten (1939-) started studies on transition metal complexes of DNA components (nucleobases, nucleosides and nucleotides) and was the first to publish crystal structures of such complexes. He later continued studying this type of compound in solution employing NMR techniques. J. Sletten (1941-), after completing her doctoral work on structure and bonding in higher homologues of thiathiophthenes, turned to the field of transition metal chemistry, with emphasis on the study of di- and polynuclear complexes showing ferro- orantiferromagnetic interaction.

Today the crystallographic facilities at the Dept. of Chemistry are excellent, with modern single-crystal and powder diffractometers. K. W. Törnroos (1956-), who came to Bergen from Stockholm U. in 1996, is presently the sole crystallographer. Törnroos has been engaged in a wide range of crystallographic projects, one of the key subjects being the study of spin-crossover phenomena.

Crystallography at the University of Tromsø



Asbjørn Hordvik and Jim King, then IUCr Executive Secretary.

The University in Tromsø was established in 1968. The pioneer in X-ray crystallography in Tromsø was A. Hordvik, who was a student of Sven Furberg while he was at the U. of Bergen. Hordvik established the first protein crystallography laboratory in Norway. He was Secretary-Treasurer of the IUCr from 1986 until

he died. The leadership of the protein crystallography group was later taken over by E. Hough and A. Smalås, and the laboratory now has status as a national centre for structural biology.

Crystallography at the University of Trondheim

In Trondheim, crystallography was studied in the Dept. of Physics at the Technical U. established in 1910 (today called the Norwegian U. of Science and Technology, NTNU). H. Brækken started the first X-ray diffraction studies of crystals in 1926, but it was H. Sørum (1915-1995) who established X-ray crystallography as a field of its own in Trondheim. He learned crystallography in the group of W. L. Bragg in 1947-1949 and received his Doctor's degree in Trondheim in 1952 on a study of some feldspars. He taught crystallography, designed equipment and did research on molecular structure, diffraction physics, disorder, defect structures, interdiffusion in metallic materials and topography at NTNU until his retirement in 1982.



Guy Fauque, Frode Mo, Michel Frey at the Lyle H. Jensen Symposium in 1986.

The best known of his students is F. Mo (1937-). He has determined accurately the structure and charge density in small organic S-containing molecules, and the structure of biologically important molecules. He has studied multiple scattering, used synchrotron radiation in materials studies, and studied structural phase transitions and ferroelectric compounds, including epitaxial thin films, under electric fields. A particularly interesting line of research was the development of the physical estimation of structure-factor phases from three-beam interference in non-perfect crystals as a novel method for initiating the determination of macromolecular structure and for studies of subtle structural changes.

In 1989, together with his colleague in the Dept. of Chemistry, D. Nicholson, Mo initiated collaboration with Swiss scientists for the purpose of constructing and operating a joint bending-magnet beamline, which later became the Swiss-Norwegian Beamlines (SNBL) at the ESRF.

In 1972, R. Høier (1938-2009) was appointed Associate Professor in Sørum's group. He was a student of J. Gjønnes in Oslo. A significant part of the work done in Høier's group was devoted to studies of metallic materials and ceramics. His main interests were in dynamic diffraction theory, many-beam effects and electron crystallography.

In 1983, E. J. Samuelsen (1937-) was appointed the successor of H. Sørum. His research has been focused on studies of the structure and properties of materials, including partially disordered materials, low-dimensional systems, in particular organic chains and layers with semiconducting properties, phase transitions, lattice vibrations and magnetism. He has used neutron-, light- and X-ray scattering in his work.

Bjørn Pedersen

The author



Bjørn Pedersen
The author of this article graduated in 1958 from Haraldsen's research group after discovering two new subsulfides of vanadium and determining the crystal structure of them. After graduation he worked for a short time as an assistant to Furberg trying to solve the structure of β-glucose. He then left the field of X-ray crystallography to work with solid-state NMR, where knowledge of crystallography also turned out to be useful, and became a professor of chemistry at UiO from 1970 to 2003 when he retired. Since then he has written articles and contributed to books on the history of chemistry in Norway.
(bjornp@kjemi.uio.no).

MEETING REPORT

High-Pressure Diffraction Frolic-Goats Workshop



Left to right: Hanna Piotrowicz, Adrián Andrada, Kamila Pruszkowska, Mehriniso Mamadjonova, Anna Olejniczak, Michał Dobrowolski, Michalina Anioła, Patryk Rzepiński, Kinga Ostrowska, Kamil Dziubek, Hanna Tomkowiak, Jędrzej Marciniak, Roland Mitletich, Doaa Abd Allah, Magdalena Kropidłowska, Mathias Meyer, Szymon Sobczak, Andrzej Gładysiak, Marcin Podsiadło, Witold Zieliński, Michał Kaźmierczak, Ewa Patyk, Ali Shaheen, Weizhao Cai, Kacper Rajewski, Michał Andrzejewski, Kristine Krukle-Berzina, Magdalena Sikora, Andrzej Katrusiak (Absent from the photo are Joanna Bąk, Anna Jenczak, Paweł Piszora, Katarzyna Salomon, Paulina Wawrzyniak).

Poznań, Poland, April 2014

The 7th High-Pressure Diffraction Frolic-Goats Workshop (FgHp-7) 2014 was held in the Faculty of Chemistry, Adam Mickiewicz U. in Poznań, Poland, 27-29 April 2014. 34 participants from 8 countries attended. FgHp-7 was designed to disseminate information on high-pressure techniques, mainly X-ray diffraction single-crystal diffractometry using a diamond-anvil cell (DAC), among crystallographers, chemists and physicists. Other techniques, such as high-pressure volumetric measurements, were presented. The lectures were focused on the methodology of high-pressure diffraction experiments and their application: 'Advancements and experimental experiences in sXRD at non-ambient conditions' (R. Miletich), 'Pressure-induced changes in pyrimidine aggregation' (E. Patyk), 'Studies on haloimidazoles' (M. Andrzejewski), 'High-pressure studies on 2,4,5-tribromo- and 2,4,5-trichloroimidazole' (K. Rajewski), 'Oscillation frequencies of molecules in liquids and high-pressure crystal structures' (J. Bąk), 'Structural and Electronic Properties in two-dimensional layered metal chalcogenides' (A. Andrada), 'Mandelic Acid *versus* the Wallach's Rule' (J. Marciniak), 'Negative area compressibility in 2-methylbenzimidazole' (W. Zieliński), 'Reversed negative linear compressibility of a nonlinear-optics organic crystal 3-methyl-4-nitropyridine N-oxide' (W. Cai) and 'High-pressure experiments and data reduction with *CrysAlis*' (M. Meyer). The *CrystEngComm* Poster Prize was awarded to H. Tomkowiak for 'Short-range interactions of organic compounds at high pressure'. The third day of the Workshop was dedicated to practical exercises on the DAC operation, alignment, loading, isochoric crystallization, and processing the diffraction data. The operation of the piston-and-cylinder press for compressibility measurements was demonstrated. The Workshop excursion and get-together were organized in Fort No. 3 (located at the centre of the New Poznań Zoo), one of 18 forts surrounding Poznań in the 19th century, then one of the largest strongholds in Prussia. The FgHp-7 Workshop was sponsored by the Faculty of Chemistry, Adam Mickiewicz U. and Agilent Technologies, and was organized by the Team supported by the Foundation for Polish Science.

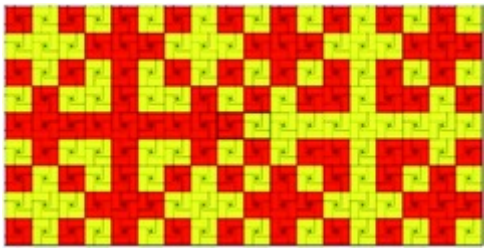
Andrzej Katrusiak

MEETING REPORT

XXIII IUCr Congress and General Assembly

Session reports continued from Volume 22, Number 4

MS34: Crystals and beyond

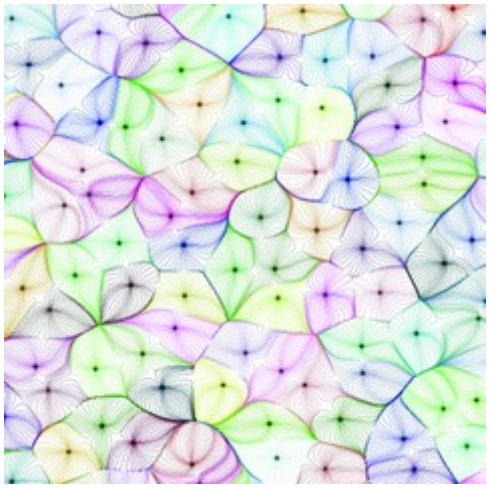


Uwe Grimm's slide showing the squiral tiling.

$$\mathrm{supp}(\gamma) \subset \Lambda(K) \quad \Rightarrow \quad \mathrm{supp}(\gamma_s), \mathrm{supp}(\gamma_0) \subset \Lambda(K)$$

Nicolae Strungaru's formula describing the main result.

This microsymposium focused on 'which structures diffract and how', including analysis of periodic, aperiodic, quasiperiodic and other structures. U. Grimm (UK) gave a general survey of aperiodic structures, their spectra and some ordered structures beyond pure-point (Bragg) diffracting crystals, such as the squiral tiling. N. Strungaru (Canada) discussed the concept of almost periodicity for measures and its connection to Meyer sets.



Robert Moody's slide showing the basins of attraction around the zeros of a Gaussian analytic function.



MS34 Speakers and Chairs (left to right): Nicolae Strungaru, Robert V. Moody, Sylvain Ravy, Lorenzo Sadun, Dominik Justel, Shelomo I Ben-Abraham, Uwe Grimm and Jeong-Yup Lee.

R. Moody (Canada) presented a form of random process in the (complex) plane arising as the set of zeros of Gaussian analytic functions and its connection to tilings and diffraction. D. Jüstel (Germany) suggested a novel form of radiation suitable for structural analysis of nanotubes, fullerenes and similar entities. S. Ravy (France) showed that coherent diffraction produces speckle patterns revealing higher order correlations undetectable by pure-point (Bragg) diffraction. As a paradigmatic example he quoted the Golay-Rudin-Shapiro sequence. L. Sadun (USA) discussed the relationship between the diffraction spectrum of a point set and the dynamical spectrum of an associated dynamical system. He also constructed a pure-point diffractive set with finite local complexity that is not a Meyer set – a counterexample to a conjecture of Lagarias

Jeong-Yup Lee and Shelomo I. Ben-Abraham

MISCELLANY

A Crystallographer’s New Year’s Poem

May you solve all your structures
May your crystals shine bright
May the beamlines keep working
All through the night

With your fingers crossed
And your loop at the ready
When you find all those crystals
May your hands be steady

A little tweaking, a lot of knowledge
And some magic vapor
Here’s hoping that this year
Nature publishes your paper!

Tom Friedlander

OBITUARY

Lip Lin Koh (1936-2015)



Lip Lin Koh, one of the most distinguished X-ray Crystallographers in Singapore, died of pneumonia on Feb 12 2015 at the age of 79. He was one of Singapore's pioneers in education, a former Dean of Science and an ex-MP of Singapore.

Koh contributed to the growth of crystallography in Singapore for more than 40 years. He organized the Inaugural Conference of the Asian Crystallographic Association in Singapore in November 1992. He was the first Singaporean to serve as a co-editor of *Acta Crystallographica* (1994-97). He championed for the Singapore National Crystal Growing Challenge as one of the judges. Koh was very active in solving and refining difficult structures for the X-ray Diffraction Laboratory and responsible for a number of related publications.

Koh graduated from Nanyang U. (Singapore) and received his PhD degree from Boston U. (USA). He taught at the Dept. of Chemistry at Nanyang U. (1964-1979) and at the National U. of Singapore (NUS, 1980-1996). He was the first Dean of Science at the NUS and served as the Head of Dept. of Chemistry and Dean of Science at Nanyang U., before the merger of the two.

After his retirement from the Dept. of Chemistry (NUS), he was engaged as a part-time research fellow at CE Resources Pte Ltd, an NUS spin-off company. He rejoined the department as an Adjunct Senior Research Fellow in 1992, offering guidance to staff and students on solving crystal structures with his expertise. He was particularly good at solving problems of disorder.

He was a member of the University council, and served as president of the Singapore Association for the Advancement of Science. From 1979-1996, Koh was an elected Member of Parliament of Singapore. He received the Public Administration Silver Medal in 1978 and the University's outstanding Science Alumni Awards in 2005.

His integrity, passion, commitment and drive will be well remembered by all who knew him. Koh will be deeply missed by NUS and Singaporean researchers, as well as by the entire Asian crystallographic community.

J. J. Vittal

MISCELLANY

Crystallography in the News



George Sheldrick

In Oct 2014 *Nature* published a list of the 100 most highly cited papers of all time. Six of the top 100 (ranked 13, 22, 23, 71, 82 and 95) concerned crystallography. At 13 on the list, George Sheldrick's 2008 paper in *Acta Cryst.* A is the highest ranking paper published in the last 20 years. Other publications describing the tools of the crystallographic trade that rank in the top 100 include *PROCHECK* (Leskowski, MacArthur, Moss & Thornton, *J. Appl. Cryst.*, 1993), the *HKL* suite (Otwinowski & Minor, *Methods of Enzymol.*, 1997), *MOLSCRIPT* (Kraus, *J. Appl. Cryst.*, 1991), the graphics program *O* (Jones, Zou, Cowan. & Kjeldgaard, *Acta Cryst.* A, 1991) and a compendium of ionic distances in halides and chalcogenides (Shannon, *Acta Cryst.* A, 1976).

An article about 87 year old Nira Rosebrough Roberts describes her career in science and the fact that she is a coauthor on the most cited scientific paper of all time (305,782 citations by Dec 2014). The paper described the Lowry method for measuring the amount of protein in solution. Her essential contribution to the work as a technician was appropriately acknowledged with co-authorship.

R. Mukhopadhyay, ASBMB Today, March 2015.



Ian Wilson

Ian Wilson, a plenary lecturer at the American Society of Biochemistry and Molecular Biology (ASBMB) Meeting in March 2015, was interviewed in the most recent *Newsletter* of the ASBMB. Ian described working on the structural biology of influenza virus, HIV and hepatitis C virus at the Scripps Research Inst. and efforts to understand how these viruses are recognized by the immune system. Ian's comments on advances in crystallography during the course of his career and his passion for structural biology included the following observations.

'The technology for X-ray crystallography just continues to improve, so the bottleneck goes back to the expression of proteins you are interested in.....My all time favorite structure, stemming from my postdoctoral work, is influenza virus hemagglutinin..... Choose a problem that you're passionately interested in but that is also challenging. If you find a good problem, you can pursue it for the rest of your life. I've been working on influenza hemagglutinin since 1977, and it's still very exciting and topical.'

Excerpted from an interview by R Mukhopadhyay, ASBMB Today, March 2015.



Robin D. Rogers

Robin D. Rogers, teacher, ionic liquids researcher, crystallographer, green chemist, entrepreneur and journal editor with the red jacket, has pulled up his southern roots and moved to Canada. Rogers has taken a position at McGill U. in Montreal, to spearhead an applied research program designed to forge partnerships with Canadian industries. At McGill, Rogers will look to help the Canadian forestry industry go beyond making paper and use nanocellulose and waste lignin to develop renewable polymeric and composite materials. He also will work with the country's commercial fishing industry to use waste chitin from shrimp and crabs. 'If properly developed, materials derived from chitin could make shrimp shells more valuable than the shrimp for food.'

Excerpted from Chemistry and Engineering News, Feb 16, 2015 by S. K. Ritter.



David Eisenberg

David Eisenberg received the ASBMB's Bert and Natalie Vallee Award in Biomedical Science. In 2005, Eisenberg's group published the first atomic-resolution structure of an amyloid fiber. Eisenberg's work enabled the development of algorithms to predict segments of proteins with high propensity to form amyloid fibers and provide useful hypotheses for amyloid-forming mechanisms in many disease-related proteins.

Excerpted from ASBMB Today, March 2015.

On July 1 2015, Janet Thornton will be stepping down from her position as director of the European Molecular Biology Laboratory, where databases for DNA sequences, protein structures and other biological data are stored. She will be replaced by joint directors Ewan Birney and Rolf Apweiler, who are already at the EBI in Hinxton, UK.

AWARDS AND PRIZES

Crystallographers honored in 2014



John Spence

John Spence, Professor of Physics at Arizona State U. and Director of Science for the US National Science Foundation's BioXEFL Center (USA) which supports applications of X-ray Free-electron lasers (XFEL) to structural biology, received the John Cowley Medal at the 18th Int'l Microscopy Congress in Prague in September.



Jenny Glusker

Jenny Pickworth Glusker, Professor Emeritus at Fox Chase Cancer Center (USA), received the Sigma Xi Procter Prize for Scientific Achievement, recognizing her ground-breaking studies of molecules involved in cancer and the Krebs cycle, and the biologically significant interactions of metal ions with proteins and ligands.



Majid Chergui

Majid Chergui, Federal Inst. of Technology (France) and editor-in-chief of the ACA/AIP Journal Structural Dynamics, received the Earle K. Plyler Prize for Molecular Spectroscopy and Dynamics from the American Physical Society for his pioneering work in ultrafast X-ray spectroscopy for studies in solution and the solid state.



Evgeny Antipov

Evgeny Antipov, Moscow State U. (Russia) and serving as ICDD ambassador to the Eastern European Community, received the 2014 McMurdie Award and Distinguished Fellow Award from the International Center for Diffraction Data (ICDD) for distinguished work that improves the Powder Diffraction File.



Jennifer Doudna

Jennifer Doudna (UC, Berkeley, USA) and Emmanuelle Charpentier (Hannover Medical School, Germany) shared the $100,000 Dr Paul Janssen Award from Pharmaceutical giant Johnson and Johnson for enabling improvements in the speed and efficiency of genome editing and uncovering molecular details of bacterial immunity mechanisms.

Excerpted from ACA Reflexions, Winter 2014, and ASBMB Today, November 2014

AWARDS AND PRIZES

The Poland–US Science Award goes to Jaskolski and Wlodawer



Alexander Wlodawer (left) and Mariusz Jaskolski (right).

The newly established prestigious award established jointly by the Foundation for Polish Science (FNP) and the American Association for the Advancement of Science (AAAS) honors pairs of collaborating scientists from these two countries. The first such award went to two macromolecular crystallographers for their studies on important proteins of medical relevance, which contributed to the development of therapies combating, among others, AIDS and leukemia. The recipients, selected from more than 50 nominations, are Mariusz Jaskolski from the Adam Mickiewicz U. and the Inst. of Bioorganic Chemistry in Poznan, Poland, and Alexander Wlodawer from the National Cancer Inst., USA. Both of them are very well known in the world-wide community of structural biologists for their high-impact publications, services on various scientific bodies, and presentations at many conferences and meetings.

Their collaboration began almost 30 years ago, when Jaskolski joined the laboratory of Wlodawer at the National Cancer Inst. and made an important contribution to the solution of crystal structures of retroviral proteases from the avian *Rous sarcoma* virus and from the human HIV-1 virus. This work paved the way for the development of successful drugs against AIDS by several pharmaceutical companies, after only 7 years of effort. As a result, AIDS is not any more a terminal disease.

After returning to Poland Jaskolski established the first macromolecular crystallography laboratory in Central Europe, and his collaboration with Wlodawer continues to this day. Among a number of collaborative accomplishments, of note is the structure solution of asparaginase, a target in the therapy of acute lymphoblastic leukemia.

Wlodawer and Jaskolski not only collaborated on a variety of research projects, but also published jointly a number of educational and instructive papers on crystallographic methods and techniques. Together, they co-authored 37 publications which to date have received more than 2,500 citations. The first FNP/AAAS prize for collaborative USA-Polish research accomplishments emphasized the importance of biocrystallography to human society. It went to a pair of highly deserving recipients.

Zbigniew Dauter

NOTICE

ACA 2015 Workshops

Philadelphia, PA, USA, July 25–29, 2015

www.amercrystalassn.org/



In addition to the full meeting program, the ACA is offering the following pre-meeting all-day workshops being held on Saturday, July 25, 2015. Pre-registration is mandatory and should be indicated on your registration form. The cost for each workshop is separate from the registration fee.

WK.01 Introduction to Modeling High-Pressure Single-Crystal Diffraction Data. The objective of this workshop is to provide a comprehensive introduction into the analysis and interpretation of high-pressure single-crystal diffraction (HP-XRD) data. The workshop will comprise a series of short lectures given by experienced high-pressure crystallographers that will provide an insight into the fundamental theory underpinning accurate HP-XRD data analysis. However, the majority of the workshop will be focused towards providing extensive hands-on HP-XRD data analysis, enabling the participant to obtain experience with the advanced features of *EoSFit* and the *Olex2* software.

WK.02 Serial Crystallography Data Analysis with Cheetah and CrystFEL: Concepts and Tutorials. Serial femtosecond crystallography has yielded several major and unique advances in structural biology previously unattainable with conventional technologies, including the potential for sub-picosecond time-resolved crystallographic studies, probing cyclic or even non-cyclic reactions. With the construction of more than a dozen new XFELs currently under way, and the multiple recent demonstrations of SFX at synchrotrons, the potential user base is growing significantly. The development and appropriate use of new software to tackle the unique problems of SFX data analysis is vital to making SFX practicable.

WK.03 Rietveld Refinement Analysis. This all-day workshop will introduce the use of the Rietveld analysis technique to the attendees. We will first emphasize the powder diffraction technique, as well as the law and rules associated with it, then move on to the Rietvield quantitative technique (solution and refinement of crystallographic data). Attendees will be asked to bring their own laptops with the software already downloaded. The workshop will be primarily targeted for novice users with limited experience in diffraction who want to gain expertise in using the Rietveld analysis technique.

WK.04 Small-Angle Scattering: Structural Biology and Soft Matter. Small-angle X-ray solution scattering continues to experience dramatic growth within both the structural biology and soft matter communities. While there tends to be relatively little interaction between these communities historically, the two share essentially the same basic theoretical foundation as well as a number of tools and techniques. This workshop will bring together leading SAS experts in both areas to prepare students for successful experiments.

For more information on the above workshops and the full program, visit www.amercrystalassn.org/.

NOTICE

ECM29

Rovinj, Croatia, August 23–28 2015

http://ecm29.ecanews.org



The 29th European Crystallographic Meeting (ECM29) will be held in Rovinj, a coastal Croatian town where subtle Mediterranean grace, traditional hospitality, rich history and culture and superb cuisine coalesce in a unique and incomparable blend. Rovinj is just 36 km away from the International Airport of Pula, while the airports of Rijeka and Trieste are about 100 km away from the town. Furthermore, Venice and Rovinj are connected by direct speedboat line. Finally, a brand new highway links Rovinj with the Slovenian border (70 km) and thus further with central Europe, as well as with the capital of Croatia, Zagreb (240 km). Located just a few steps away from the historical city centre, within walking distance of the majority of hotels, the city port and the central bus station, the conference centre will be an adapted old tobacco factory complex, the Adris exhibition and convention centre.

More than 700 abstracts have been submitted up to now. The Presenting Authors' registration deadline is May 23 2015, while the Regular registration deadline is August 7 2015. The Organizing Committee with its partners will make every effort to ensure the safety and well-being of all ECM29 participants. All visitors from EU/EEA countries are allowed to enter Croatia with their valid ID cards or passports, and citizens of many countries outside EU/EEA can enter Croatia without a visa. Please follow the news on ECM29 at http://ecm29.ecanews.org and on social networks. We are looking forward to seeing you in Rovinj

Aleksandar Višnjevac and Mario Cetina