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Contents

> Extraction incomplete: missing article positions 1.

IUCr journals news

Michael Levitt – The Nobel Prize in Chemistry 2013 3

Regional news

On the rise: popularity of science in the UK 5

ACA History Website Adds 'ACA Beginnings' 43

IYCr 2014

2015: Crystallography matters ... more! 7

The IUCr needs you! 10

Pan African Meeting and Summit of the International Year of Crystallography 12

Bruker OpenLab Morocco 16

Rigaku OpenLab Cambodia 18

PANalytical OpenLab Mexico, 18–21 November, 2014 21

Agilent OpenLab Hong Kong, 3-7 December, 2014 23

Meeting report

3rd China-India-Singapore Conference on Crystal Engineering 20

XXIII IUCr Congress and General Assembly 26

Crystallographic Society of Japan 38

Heart of Europe Bio-Crystallography 40

IUCr activities

Report from Executive Committee 36

New IUCr Commission on NMR Crystallography and Related Methods 41

Awards and prizes

PANalytical Award supports young scientists 44

Notice

ECM 2015 45

Zurich School of Crystallography 2015 46

IUCR JOURNALS NEWS

Michael Levitt – The Nobel Prize in Chemistry 2013



Michael Levitt

The Nobel Prize is an international award administered by the Nobel Foundation in Stockholm, Sweden. It has been awarded every year since 1901 for achievements in physics, chemistry, physiology or medicine, literature and for peace. Over the course of its history, many awards have been made for scientific achievements directly related to, or involving the use of, crystallographic methods and techniques.

Michael Levitt, FRS, is a biophysicist, IUCr author and professor of structural biology at Stanford University, CA, USA, a position he has held since 1987. Levitt, together with Martin Karplus and Arieh Warshel, received the 2013 Nobel Prize in Chemistry for 'the development of multiscale models for complex chemical systems'. In the field of structural analysis, Levitt and his co-workers have been instrumental in mimicking and predicting the behaviour of molecules using computers. An example is his work in modelling the structure of protein molecules *in silico* to answer complex questions concerning the role of amino acids in protein structure.

In 1967 Levitt gained a BSc in physics from King's College, London, England, and through true grit and determination won a place at the Laboratory of Molecular Biology, Cambridge University, England, to study for his doctorate in biophysics. Levitt spent a year at the Weizmann Institute in Israel before taking up his studies in Cambridge. Whilst in Israel, Levitt started to work in the then brand new field of computational structural biology as a programmer for Warshel and Shneior Lifson, writing the first program for simulation of protein motion by energy minimization.

It was John Kendrew who sent the young Levitt to Israel to work with Lifson on how to use potential energy functions and computer simulations to calculate the properties of macromolecules of biological interest, giving Levitt a running start during his PhD studies, as by the time he started in 1968 he had already written the first program to move the atoms of a protein by minimizing an empirically calibrated potential energy function. Levitt's PhD thesis was entitled 'Conformational Analysis of Proteins'. It described the basic form of the energy function, different coordinate systems and energy minimization, before introducing a method for deriving a potential energy function that stabilized the known X-ray structure of a protein molecule. It then used this potential to energy refine protein structures by moving atoms so that they fit stereochemical laws, to interpret problematic regions of electron-density maps, to examine the transition state in the enzyme action of lysozyme and to examine the tertiary structure changes occurring in haemoglobin.

Levitt was awarded his PhD in 1971, and the following year he took up a postdoctoral fellowship at the Weizmann Institute. In 1974 he moved back to the MRC Laboratory of Molecular Biology at Cambridge to work as a staff scientist. Levitt spent a couple of years as a visiting scientist with Francis Crick at the Salk Institute, La Jolla, CA, USA. In 1979 he became Associate and Full Professor of Chemical Physics at the Weizmann Institute. He was a visiting scientist at the MRC Laboratory of Molecular Biology, Cambridge, between 1986 and 1987, and in 1987 he moved to the USA to become Professor of Structural Biology at Stanford University.

Levitt's early work set the stage for most of what he and the field have been doing since. In the last 45 years computing has become less expensive by at least ten-million fold. Computers now dominate all walks of life, and biology has become an information-rich science. These developments were instrumental in simulating movement by Newton's second law as the power of the computer could model literally billions of iterations. The same methods are also applied to proteins, RNA and DNA and they can also be used to refine structures against NMR and X-ray data.

To this very day Levitt is still inspired and involved in many of the structural methods he and co-workers pioneered. For example, one aspect of his research focuses on the combined use of mass spectrometry, cryo-electron microscopy and *R*-value exploration of X-ray data with computer methods that allow large macromolecular complexes to be solved with less information.

One of Levitt's recent papers published with the IUCr looks at membrane proteins and large protein complexes that are notoriously difficult to study with conventional X-ray crystallography methods, not least because they are often very difficult, if not impossible, to crystallize, but also because their very nature means they are highly flexible. The result is that when a structure can be obtained it is often of low resolution, ambiguous and reveals a mosaic-like spread of protein domains that sometimes create more puzzles than they solve.

Levitt and co-workers have reviewed their earlier refinement technique known as Deformable Elastic Network (DEN) and found ways to optimize it successfully for the investigation of several particularly problematic protein structures, including soluble proteins and membrane proteins up to a resolution limit ranging from 3 to 7 Å [Schröder, Levitt & Brunger (2014). *Acta Cryst.* D**70**, 2241–2255; doi: http://doi.org/zm7].

The team explains that advances in X-ray technology and light sources have in recent years led to structures for previously intractable proteins such as the ribosome, transcription complexes and even viruses. The details then lie in a successful refinement that can provide valuable information about the structure in question despite lower resolution than would normally be desirable. 'The interpretation of low-resolution diffraction data is generally difficult', the team says, 'owing to the unfavorable ratio of parameters (variable degrees of freedom, such as flexible torsion angles or Cartesian atomic coordinates) to observables (observed diffraction intensities).' Ambiguities and errors of interpretation abound.

The DEN approach begins with a model, a prediction, of the target structure containing as much information as is known ahead of the insertion of the diffraction data, and determines which features of the model ought to be adjusted to fit the diffraction data emerging from the X-ray experiments. In other words, a null hypothesis is applied; those parts of the model not predicted to alter the diffraction data are retained as is. Distances between randomly chosen pairs of atoms within the structure are tested and fine-tuned accordingly within a distance restraint, customarily referred to as the elastic network.

Alongside many friends, mentors and colleagues (such as John Kendrew, Max Perutz, Francis Crick and Aaron Klug), Levitt feels the computer industry has also played an instrumental role in being able to accomplish all that he has.

'Computers and biology go together. Biology is very complicated, and computers are such wonderful, powerful tools. And they just keep getting more and more powerful.'

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

REGIONAL NEWS

On the rise: popularity of science in the UK



In the UK at least, year on year we are seeing more people likely to enter higher education. Across the UK, 18 year olds became more likely to enter higher education in 2013 than ever before; a staggering 40% of young people in England now go on to higher education by the age of 19. Amongst these numbers, more students now are opting to take science-related degrees at university. This trend is also filtering through to our nation's schools, which also show a rise in interest from 5–18 year olds.



Budding scientists at the British Crystallographic Association/Science and Technology Facilities Council stand at The Big Bang Fair 2014 in Birmingham in March.

The latest results can be found in the UCAS 2013 Application Cycle: End of Cycle Report (www.ucas.com/sites/default/files/ucas-2013-end-of-cycle-report.pdf). The results are certainly welcome and confirm the rise in popularity seen in the general media for science and engineering features.

Outreach activities in 2014 such as The Big Bang Fair (www.thebigbangfair.co.uk) have all contributed positively to the popularity of science and engineering. The Big Bang Fair is the largest celebration of science, technology and engineering for the young in the UK, with a target audience of students aged between 7 and 19. The event aims to show how exciting and rewarding an interest and career in science can be.

With the increased interest in science within schools and universities, we should anticipate greater demand for certain core areas of science teaching such as crystallography to increase again. The challenge to grow the degree of crystallography taught in our schools, colleges and universities is incumbent on all of us, and at the IUCr we are extremely keen on championing any efforts to engage with the community to this end.

The IUCr Crystallographic Teaching Commission is one of several IUCr Commissions and is responsible for supporting activities relating to the teaching of crystallography. It was established at the Third General Assembly with the objective of exchanging information on an international scale on the subject of teaching crystallography, of promoting publication of articles on teaching and for arranging discussions.

To maintain this surge in interest in the science, technology, engineering and mathematics (STEM) disciplines, it is more vital than ever to create a support network for schoolchildren to encourage them to engage with science and engineering at an early stage to help them become career scientists and engineers as they grow older. I feel this presents a challenge to all of us to help educate and promote, a challenge I am sure we will all embrace with enthusiasm.

Schemes such as the Participatory Research CPD programme (www.sciencemuseum.org.uk/educators/teacher_cpd_and_events/research_cpd.aspx) go a long way to engaging with our young, and inspiring them to think about careers within the science discipline. The programme is run by experienced educators from the Science Museum with researchers from King's College London. Together they explore and refine ways of integrating students' home-life experiences and personal interests into approaches that will build science capital and ultimately improve students' science aspirations.

Sadly, we still face a number of worrying issues and claims over poor levels of science literacy and teaching levels in our schools. The UK Government is reforming AS- and A-level qualifications to ensure they are academically rigorous, and provide students with the knowledge and understanding to prepare them for higher education and employment.

Another recent step has seen Government strategy published that sets out plans to stimulate economic growth by supporting science and innovation. The Government's science and innovation plan will reduce the barriers to business-led innovation.

This heightened interest in science is an opportunity to bring our best brains to the fore and discuss with our next generation of scientists the challenges facing both the environment and industry at large. We must not only inform but also encourage debate; this will ensure we build on the growing interest in science and tackle head-on some of the disconnect between the degree of science teaching in our classrooms and resources open to our young students.

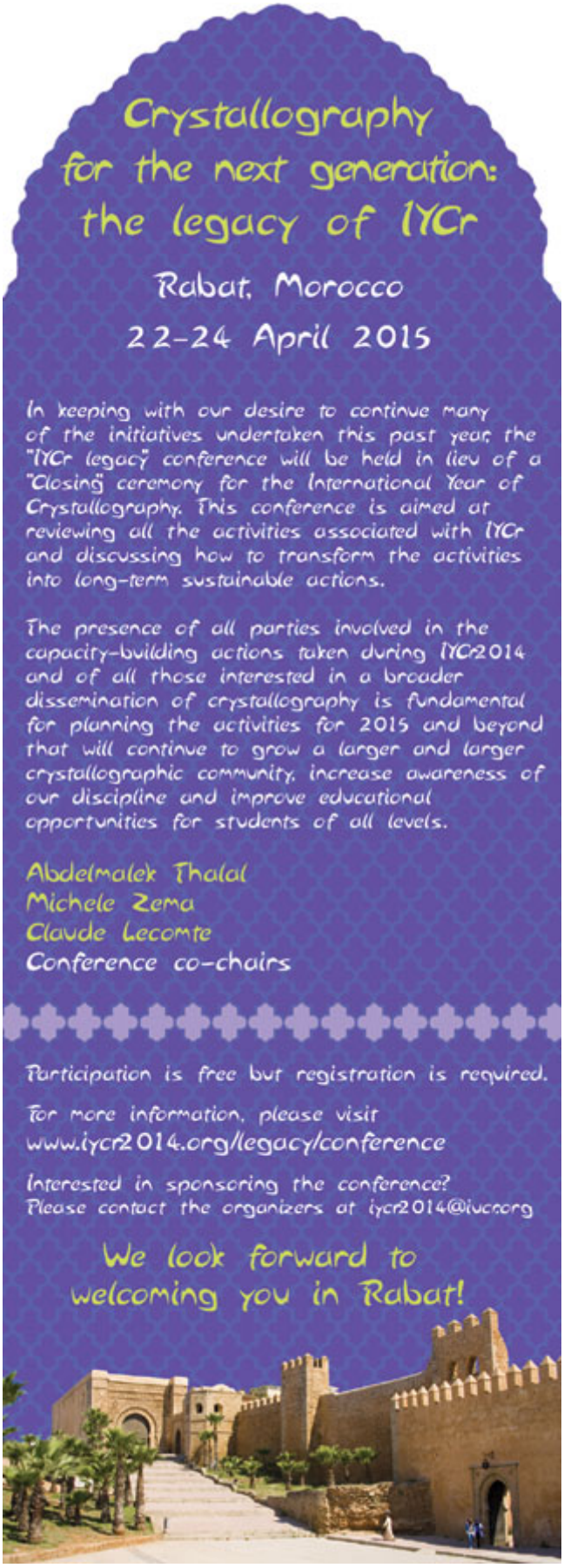
The future can be a bright one for science providing we continue to build the infrastructure in our communities, and awareness and interest in our schools and colleges.

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

IYCR 2014

2015: Crystallography matters … more!





The year 2014 has inevitably come to an end and, with it, the UN International Year of Crystallography is formally closed. It has been a hectic, exciting and stimulating year. IYCr2014 was started with a booklet

entitled 'Crystallography matters!', produced with UNESCO and translated into 15 languages. After all the initiatives for IYCr2014, it is hoped, Crystallography now matters … *more*!

The IUCr, all the regional and national associations and many individual crystallographers have worked hard to reach the declared goal of raising awareness in the world at large about the importance of crystallography in the modern world. Through an incredible variety of activities worldwide, that objective has been brought to life for thousands of schoolchildren, university students and the general public. In the past year, many initiatives have been started by the IUCr, partnered by UNESCO, supported by industrial and academic sponsors, and made real by a host of willing volunteers. They have ranged from science fairs and crystal-growing competitions for schoolchildren, through professional-level OpenLab workshops and training sessions, to international summit meetings to shape future policy and bring nations together through science. They have ignited a fire in the new generation, most especially in parts of the developing world where structural science is still an infant science. We expect the audiences of students and young teachers who attended these events to now act as 'nucleating agents' in their countries and continue to grow and nurture the crystallographic community.

To build on these successes, the IUCr is embarking on an ambitious set of new initiatives to ensure that this newly kindled flame does not go out: more OpenLabs will be commissioned; more sustained efforts will be made in capacity building; more effort will go into public outreach activities. To pursue such objectives and enable the continuation of many initiatives successfully launched during IYCr2014, an 'IYCr legacy' fund has been established (see article The IUCr needs you!).

A conference entitled *Crystallography for the next generation: the legacy of IYCr* will open this new chapter for the crystallographic community (see right). It will be held at the prestigious venue of the Hassan II Academy of Science and Technology of Morocco in Rabat on 22–24 April, 2015. This is a very fitting venue as the Moroccan community was instrumental in gaining approval for IYCr2014. The 'IYCr legacy' conference will be held in lieu of a 'Closing' ceremony for IYCr to strengthen the message that IYCr has been a starting point for new initiatives that the IUCr will try to continue as sustainable long-term initiatives.

I look forward to meeting you all in Rabat.

Michele Zema (mz@iucr.org)
IUCr Project Manager for IYCr2014

IYCR 2014

The IUCr needs you!



Photo courtesy of Sem Gorfman and Mohamed Ateya.

Even though IYCr2014 is over, we are committed to continuing the excellent work and outreach initiated by you during the year. To help achieve this goal we have created the **IYCr2014 Legacy Fund** (www.iycr2014.org/legacy).

The aim of the IYCr Legacy Fund is to support the following:

to continue promotion of the fundamental role crystallography plays in the different branches of science, including chemistry, mineralogy, physics, biology, medicine, materials science, cultural heritage and geosciences;

to target governments by interacting with them and advising on the design of policies that will support the establishment and operation of crystallography teaching, ranging from modernising existing crystallography teaching material in schools and universities to developing closer collaborative ties with crystallography centres across the world as well as synchrotron and other large-scale facilities;

to continue to increase awareness of the way crystallography underpins most of the technological developments in modern society, and also its role in art and cultural heritage, *via* public conferences, sponsorship of poster exhibitions highlighting the usefulness and marvels of crystallography and by the commissioning and submission of articles to the press, television and other media on the contribution crystallography makes to the global economy.

'*Of course, a lasting legacy from the International Year of Crystallography is not just related to outreach activities taking place during the year. It is also about creating lasting initiatives in our schools, colleges, universities and other places of learning to continue the message about the importance of crystallography. We want to see a nation of youngsters being inquisitive about crystallography and governments enabling schools and colleges with opportunities to teach crystallography alongside the core science disciplines currently featured. This can't happen overnight; however, with the launch of the IYCr Legacy Fund we stand a real chance to accomplish these goals, by continuing many of the initiatives launched during the Year*'. Peter Strickland, Executive Managing Editor, IUCr.

A major initiative of IYCr2014 was to promote international cooperation and capacity building through the OpenLab scheme (www.iycr2014.org/openlabs). We will continue with the successful OpenLab program in 2015; if you would like to suggest a new OpenLab, please contact Michele Zema, IYCr2014 Project Manager at mz@iucr.org. OpenLabs are a network of operational crystallographic laboratories based in different countries worldwide, many in less endowed regions of Africa, South and Central America and South Asia. They are aimed at allowing access to crystallographic knowledge and technology in all parts of the world, key for the fruitful development of science, and to open possibilities for conducting high-level research.

Another highly successful event that took place during IYCr2014 (September 10–19) was the IUCr-UNESCO OpenFactory (www.iycr2014.org/openlabs/grenoble-darmstadt) with the sponsorship and active

participation of STOE, DECTRIS and Xenocs. It brought together 20 young scientists from 15 different countries in an intensive and stimulating training programme in theoretical and practical aspects of X-ray crystallography and small-angle X-ray scattering. The participants had the opportunity to discuss recent research results, learn from highly experienced XRD users, and build up networks. After ten days of intensive learning, the young scientists and guest scientist left having made new friends and collaborative partnerships for the future. If you were involved in the OpenFactory or would like to organise a new event, please get in touch with Jonathan Agbenyega, IUCr Business Development Manager, at ja@iucr.org.

A number of projects aimed at capturing the imagination of schoolchildren were launched around the exciting science of crystal growing. Materials for a crystal-growing competition were supplied to selected schools belonging to the UNESCO Associated Schools Network. The IYCr2014 website (www.iycr2014.org) was used to catalogue a number of existing national or regional crystal-growing competitions, and to provide materials, educational videos and guidelines to encourage the start of new competitions, to continue well after the International Year draws to a close. Please contact Jonathan Agbenyega at ja@iucr.org if you would like to run or be involved in organising a crystal-growing competition in your region.

A paper entitled 'IYCr2014: Spreading the Word About Crystallography in an International Year' by Brian McMahon and Michele Zema of the IUCr (http://tinyurl.com/ACS-DivCHED-CCCE) describes in more detail activities that have taken place throughout the International Year.

There can be no doubt that the International Year has celebrated the success of modern crystallography, and has set in motion several initiatives to make it a subject known to and understood by a new generation and new students worldwide. We look towards you – our many friends and colleagues – to keep the flame we created in 2014 for crystallography glowing ever brightly. We hope you will join with us as, Crystallography matters … more!

To donate to the IYCr Legacy Fund, please go to www.iycr2014.org/legacy/legacy-fund

IYCR 2014

Pan African Meeting and Summit of the International Year of Crystallography

Bloemfontein, October 12–17, 2014



Delegates at IYCr2014Africa.

In celebration of 2014 as the International Year of Crystallography (IYCr2014) as declared by the United Nations General Assembly (UNGA; resolution A/RES/66/28), the IUCr hosted three world summit meetings during 2014, *i.e.* in Karachi (Pakistan), Campinas (Brazil) and Bloemfontein (South Africa).

The third world summit of the IYCr (in Africa) was hosted at the U. of the Free State (UFS) in Bloemfontein, South Africa, by Andreas Roodt, Head of the Dept. of Chemistry and President of the European Crystallographic Association (ECA). It had the ambitious theme of 'Crystallography as vehicle to promote science in Africa and beyond', and consisted of a 2.5-day conference (Oct. 12–15), followed by a 2-day summit (Oct. 15–17).

Financial support for the event was secured from the South African Government's Dept. of Science and Technology, the IUCr, the South African Agency for Science and Technology Advancement (SAASTA) *via* the South African National Research Foundation, and UFS Chemistry.

This Pan-African Meeting of the IYCr was attended by more than 100 senior researchers, early career researchers, postdoctoral fellows and students representing more than 40 research groups from 32 universities and 22 countries, primarily from Africa and Europe, and included decision makers. All the delegates were in agreement that there is a clear sub-optimal level of regional collaboration in science which requires immediate action, and the view was expressed that supporting the broad discipline of crystallography will significantly contribute to promoting science in general.



African representatives at IYCr2014Africa.

The meeting welcomed delegates from across Africa, including a number of presidents and representatives of African Crystallographic Associations, and aimed to showcase the current state of crystallography on the continent. Among those attending were Thomas Auf der Heyde, the acting Director-General of the Dept. of Science and Technology (South Africa); Gansen Pillay, acting CEO of the National Research Foundation (South Africa); Jean-Paul Ngome Abiaga, International Basic Sciences Program, UNESCO (Paris, France); Prosper Kanyankogote, Vice-chancellor, U. of Kinshasa (DRC); Santiago Garcia-Granda (Oviedo, Spain), representative of the Executive Committee of the IUCr; Michele Zema (IUCr/Pavia, Italy), Project Manager of IYCr2014; Abdelmalek Thalal and Habib Boughzala, Presidents of the Moroccan and Tunisian Crystallographic Associations, respectively; and Petrie Steynberg (Sasol Industry, South Africa).



Keynote speakers and decision makers at IYCr2014Africa.

At the conference, the focus was on the discussion of the current state of crystallography in Africa, in particular as presented in 15 keynote lectures, but also in lectures by some 15 young scientists from the English-, French- and Arab-speaking African countries. There was also ample time for presentation of research at poster sessions by students and young scientists, and selected poster presenters had the opportunity to present their work in short 'flash' presentations.

A number of crystallographic research areas were covered, including powder diffraction, small-molecule chemical crystallography, biological crystallography, industrial crystallography, mineralogy, electron microscopy, surface crystallography, materials science and (limited) synchrotron work.



South African icons honored; from left: A. Roodt (host IYCr2014Africa), Jan Boeyens and Luigi Nassimbeni.
Two South African icons, Jan Boeyens (U. of Pretoria) and Luigi Nassimbeni (U. of Cape Town), were also honoured for their contributions towards crystallography over the past number of decades.

At the Summit, the focus was on how to utilize crystallography as a vehicle to expand science in Africa, with inputs from established and young scientists and policy makers. Two panel discussion sessions between young scientists on the one hand and senior decision makers on the other yielded an interesting discourse.



First signatories of the Declaration at IYCr2014Africa.
Highlights of the Summit were the issuing of a Declaration to decision makers in the international science arena such as the IUCr and UNESCO and in Africa and Europe, signed by 73 individuals, and the establishment of a steering committee to cement the formation of an African Crystallographic Association. The steering committee currently has representation from 18 African countries and envisages the expansion thereof in the immediate future.

Key points put forth in the Declaration were to:

- pro-actively continue with programs to ensure that the legacy of the International Year of Crystallography, particularly the promotion of science, is preserved;
- over time provide basic diffraction equipment for crystallographers in all countries in the region to allow research activity in crystallography and balanced partnership collaboration across Africa and beyond;

- facilitate the establishment of National Committees of Crystallography in African Countries and support the activities of the existing ones;
- introduce a scientific visa to ensure mobility of researchers between African nations. Such a visa would allow for the exchange and collaboration between African countries and the sharing of scientific resources and expertise, to address common developmental targets, for the benefit of all. This scientific visa should be free of charge, be valid for at least a year, and should be issued quickly once certified by appropriate higher education and research bodies;
- support training workshops and promote joint research projects;
- encourage the mobility of researchers within the region;
- leverage national bodies, institutions and international funding agencies for financial support;
- facilitate regional conferences on the subject of crystallography and its applications in Africa;
- assist in the promotion of crystallography and science in education programs;
- provide the very poor countries with minimal infrastructure and materials for research such as powerful computers and servers for data analyses;
- assist in creating a database, listing African crystallographers;
- establish a public awareness and engagement program that will create fact-based understanding of crystallography through awareness, dialogue and education in the region.

Moreover, the establishment an African IYCr Cooperation Fund, facilitated by the IUCr and UNESCO, was also proposed, which is envisaged to support actions such as:

- increasing collaboration and cooperation among scientists in Africa;
- providing seed money for up to two projects per annum involving a minimum of two countries in the region, of which at least one should be well established in crystallography;
- funding for short-term visits of up to 3 months for early career researchers;
- supporting training workshops at established centres of crystallography or at emerging centres in the region;
- enabling the sharing of facilities within the region.

The overarching feedback from the meeting was positive but it was also unanimous that more interaction between African colleagues is urgently needed to expand on the ambitious theme, *i.e.* to indeed 'use Crystallography as a vehicle to expand science in Africa and beyond'.

Andreas Roodt and Michele Zema

IYCR 2014

Bruker OpenLab Morocco

26 May to 20 June, 2014



Map of northern Morocco, showing the three OpenLab locations.

The IUCr-UNESCO OpenLab Morocco, organized in partnership with Bruker France, was held as a travelling lab making use of Bruker portable instrumentation (an X2S single-crystal diffractometer and a D2 powder diffractometer). Three stops were made, the first in Rabat, then El Jadida and finally Agadir. The overall local organization was done by the Moroccan Crystallographic Association (AMC).



The travelling lab at its first stop in Rabat.

The first stop at the Faculty of Sciences, U. Mohammed V-Agdal in Rabat on 26–30 May, 2014, was attended by 36 PhD students and postdocs from the Universities Moulay Ismaïl Meknès, Mohammed V-Agdal Rabat and Hassan II Casablanca. Students were selected from a long list of applications based on their CVs by the scientific committee. Besides the IUCr and Bruker, the OpenLab in Rabat was supported by the Faculty of Sciences, the U. Mohammed V-Agdal and the company Radaco. Lahcen El Ammari and Mohamed Saadi chaired the local organizing committee. The OpenLab was opened by Abdelmalek Thalal (U. Marrakech, President of the AMC), who also gave a lecture on crystal symmetry. Lectures and hands-

on tutorials were held by professors from different Moroccan universities (A. Aatiq, S. Benmokhtar, M. Berraho, A. Boukhris, A. Brittel, L. El Ammari, A. El Bouari, A. Laknifli, M. Saadi, K. Yamni and D. Zakaria), together with Loïc Le Dréau from Bruker France and Michele Zema from the IUCr.



Group photo at the second stop in El Jadida.

The travelling lab made its second stop at the U. Chouaïb Doukkali in El Jadida from 9–11 June. Also in this case, 36 PhD students and postdocs from El Jadida, Casablanca, Fez, Tangier, Agadir and Meknès attended the training courses, held by eight of the lecturers and instructors mentioned above, from El Jadida, Casablanca, Rabat and Marrakech, as well as Loïc Le Dréau from Bruker France. The local organizing committee was chaired by Driss Zakaria, and the OpenLab received support from the Faculty of Sciences and the University.



Participants at the last stop in Agadir.

The third OpenLab, locally organized by A. Boukhris, was held on 16–20 June at the U. Ibnou Zohr in Agadir and attended by 70 PhD students and postdocs from Morocco, Algeria and Tunisia. In addition to financial support from the IUCr and logistical support from Bruker, the University contributed financial, human and material resources. As at the other venues, the programme began with formal speeches followed by lectures on crystal symmetry, X-ray diffraction, refinement and structure solution and data collection, and practical training on the diffractometers from some of the aforementioned lecturers and instructors together with M. Belhachemi.

The gender split across all three OpenLabs was 70% male and 30% female.

Lahcen El Ammari and Mohamed Saadi (Rabat), Driss Zakaria (El Jadida) and Abdelmalek Thalal (Marrakech)

IYCR 2014

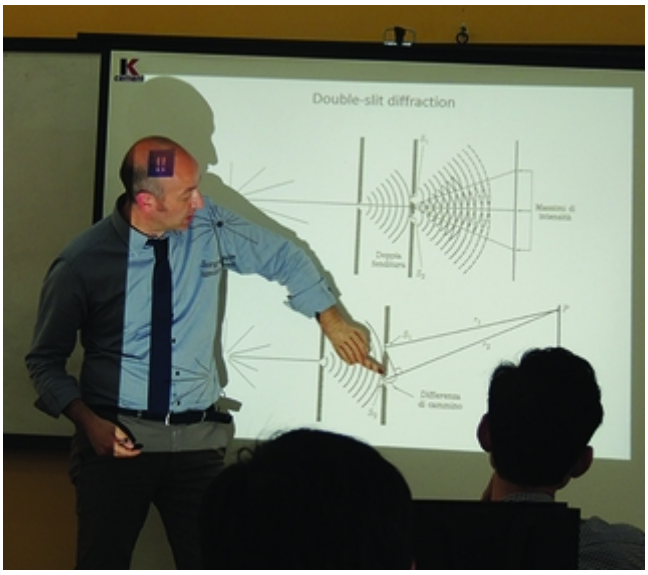
Rigaku OpenLab Cambodia

7–11 July, 2014

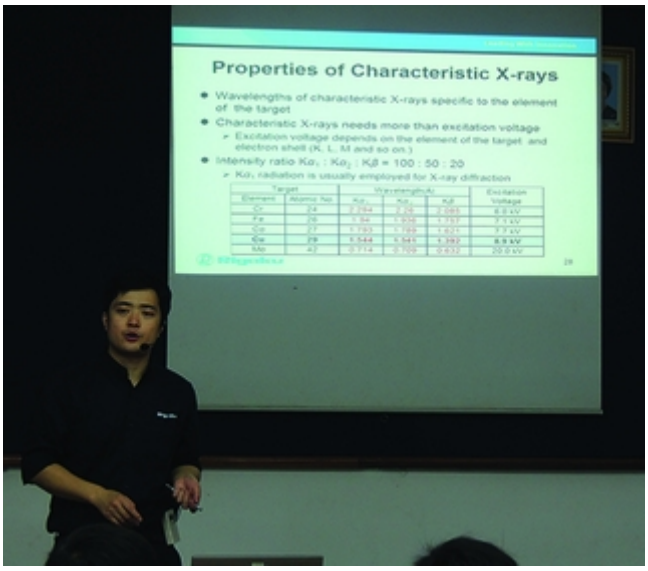


Opening ceremony.

Since mid-2013, when a Rigaku MiniFlex X-ray diffractometer was installed at the Dept. of Georesources and Geotechnical Engineering (GGE) at the Inst. of Technology of Cambodia (ITC) in Phnom Penh, the students in the department have been introduced to X-ray diffraction and crystallography. To increase their knowledge, the first IUCr-UNESCO OpenLab in Cambodia was held at the ITC in conjunction with IYCr2014 from July 7 to 11, 2014.



Lecture by Dr Zema on symmetry and diffraction.



Lecture by Dr Bing on X-ray powder diffraction.

Organized by the GGE Dept. in partnership with Rigaku, the workshop focused on the powder diffraction technique and its applications, making use of the MiniFlex diffractometer. The 22 participants included students at the ITC, Universiti Sains Malaysia and Universitas Gadjah Mada in Indonesia (undergraduates and postgraduates) and young scientists working in the public (Ministry of Mines and Energy and of Industry and Handicraft) and private sectors (mining company and cement industry) in Cambodia.

The Opening Ceremony on Monday, July 7, was chaired by Kim Ngun Bun (lecturer at ITC and local organizer of the event), and welcome speeches were given by Phol Norith (Deputy Director of ITC), Kazuyuki Inoue (Rigaku Corporation), Ros Soveacha (UNESCO Cambodia) and Michele Zema (IUCr, Project Manager for IYCr2014). After the opening remarks, Dr Bun gave a talk about research activities and perspectives in Cambodia and at the ITC in particular. Dr Zema then introduced the global IUCr-UNESCO OpenLab project and the worldwide activities taking place during IYCr. The afternoon was dedicated to the basics of symmetry and diffraction taught by Dr Zema. On the second and third days, Yue Bing (Rigaku Corporation) introduced the topic of X-ray powder diffraction, including systems, methods and instrumentation. The last two days were dedicated to hands-on tutorials including sample preparation and data analysis. Students were able to collect powder diffraction patterns from their own samples and analyze the data. Various specimens such as rocks, ceramics and metals were used during this section.

At the end of each day of training, the participants were requested to complete a questionnaire. Certificates were awarded to the participants at the Closing Ceremony by Dr Zema. The participants were very enthusiastic about the OpenLab activity and this could promote knowledge of crystallography in Cambodia.

Kim Ngun Bun, Local Organizer

MEETING REPORT

3rd China-India-Singapore Conference on Crystal Engineering

Bangalore, India, 8–10 December, 2014



The 3rd China-India-Singapore Conference on Crystal Engineering was conducted successfully at the Indian Institute of Science, Bangalore, between 8 and 10 December 2014. This meeting was held as part of the IYCr2014 celebrations and was supported by the Department of Science and Technology. The Royal Society of Chemistry, the American Chemical Society and the IUCr also supported the meeting.

There was a special session on journals where the role of **IUCrJ**; *Acta Crystallographica Sections B*, *C* and *E*; *Crystal Growth & Design* and *CrystEngComm* on the one hand and the *Journal of the American Chemical Society* and *Angewandte Chemie* on the other were highlighted. Many senior editors of one or more of these journals were present at the meeting.

In keeping with the broad theme of IYCr, it has been decided to morph this meeting into the South and East Asia Conference on Crystal Engineering (SEACCE) and include countries like Bangladesh, Malaysia, Nepal, Pakistan, Sri Lanka, Thailand and Vietnam. This development is very much in adherence with the idea of bringing nations together through science.

It is proposed to hold the next meeting in 2016 in Nepal or Bhutan, which are neutral territories, thereby facilitating the attendance of a large number of workers in our politically sensitive region.

Gautam R. Desiraju

IYCR 2014

PANalytical OpenLab Mexico, 18–21 November, 2014



Training on the new equipment.

To celebrate IYCr2014, the Instituto de Geología (IGEOL) of the Universidad Nacional Autónoma de México (UNAM) has made an important effort to modernize its crystallographic facilities by acquiring a new multipurpose diffractometer that will join the two existing diffractometers in the X-ray Diffraction Laboratory at the Institute. New computing facilities and crystallographic software have also been acquired.

To raise awareness of the existence of this infrastructure at the national level and the potential that crystallography has to solve problems in different areas of knowledge, IGEOL organized a four-day OpenLab lasting from 18 to 21 November within its facilities at Mexico DF. The OpenLab was intended for postgraduate and postdoctoral students, and attracted 60 participants mostly from Mexico but also from other Latin-American countries.

The OpenLab was organized by the X-ray Diffraction Laboratory of the IGEOL, assisted by Fabián Durán, coordinator of Communication Science IGEOL. We invited speakers from UNAM and other research centers, as well as PANalytical technicians who offered practical training on the new equipment. The program included several lectures on the fundamentals of X-ray diffraction and on the applications of crystallography in gemology (Juan Carlos Cruz Ocampo), in cultural heritage (Xim Bockimi), in the fabrication and characterization of new materials (Marius Ramírez and Martín Hernández Landaverde), in the cement industry (Jorge Pablo González), in environmental geochemistry (Mario Villalobos Peñalosa), in biomineralization (Ábel Moreno Cárcamo), in crystal growth (Héctor Riveros Rotgé), in mineralogy (Oscar Irazaba Ávila and Teresa Pi Puig) and in ore genesis (Teresa Pi Puig). The president (José Álvaro Chávez Carvayar) and former president (Lauro Bucio Galindo) of the Mexican Society of Crystallography (SMCr) delivered lectures on the activities undertaken in Mexico during IYCr2014 and on the future of the SMCr and the Latin-American Crystallographic Association.



Crystallization workshops for children.

Two public outreach activities also took place, namely the screening of the film 'The Mystery of the Giant Crystals' and a lecture on Crystallography and the Origin of Life, both delivered by Juan Manuel García-Ruiz from CSIC-U. of Granada (Spain). On the afternoon of Wednesday, November 20, participants visited the Museum of Geology, a beautiful historical museum built during the early years of the last century. During the visit, guided by the team of the Museum (Luis Espinosa Arrubarrena and Julio Caballero Corona), the participants were able to witness the crystallization workshops for children offered from this year onwards by the Museum with the help of the X-ray Diffraction Laboratory team (Fernando Núñez Useche and Adriana Gómez Cruz).

During IYCr2014, the X-ray Diffraction Laboratory of UNAM has participated in two other outreach events, namely 'Encounter with the Earth' and the 'Sciences and Humanities Party', which both saw a large and enthusiastic participation from children, teens and families.

The workshop ended with the poster-prize ceremony. From the 20 posters presented, an international jury selected two prizes for graduate students, awarded to Guillermo Dolores Reyes and Laura Esmeralda Mendoza Ramos, and two prizes for Master and PhD students, awarded to Serafín Sánchez Pérez and Luisa María Mainou. During the OpenLab, the participants enjoyed excellent Mexican cuisine created by the Romero family.

According to UNESCO, Mexico has a shortfall of experts in earth sciences and crystallography so IGEOL intends to continue offering new courses to produce experts in both disciplines with good job opportunities.

Teresa Pi Puig, Local Organizer

IYCR 2014

Agilent OpenLab Hong Kong, 3-7 December, 2014



Participants at the IYCr2014 OpenLab Hong Kong, HKUST, 3-7 Dec., 2014. Photo credit: Herman Sung.
The OpenLab was held over five days on 3-7 December, 2014, at the campus of the Hong Kong U. of Science and Technology (HKUST), Clear Water Bay, Kowloon, China. A total of 38 participants were registered, with 20 from outside of Hong Kong, including Philippines (6), China (5), Thailand (4), Malaysia (3) and India (2), and 18 from four universities within Hong Kong. In addition, there were six speakers (Fraser White of Agilent Technologies, Oxford, UK; Horst Puschmann of OlexSys, Durham, UK; Birger Dittrich, U. Hamburg, Germany; and Alison Edwards, Bragg Inst., ANSTO, Australia, as well as Prof. Williams and Prof. Zema). Four local helpers (Herman Sung, Lawrence Wong, Yan Zhou and Gemma Tam) also assisted with the laboratory demonstrations and crystallization exercises.

The theme of the OpenLab was a Small-Molecule Chemical Crystallography school, and whilst most participants had some practical or working knowledge of the experimental method of crystallography, their theoretical background was lacking. Some attempts were made to initially separate the school into a class of advanced participants and a class of beginners, but after one or two sessions it was felt the participants could be best handled and would gain the most together. The lecture material was augmented by practical work on the participants' own laptop computers with programs such as *Olex2*. In addition, evening sessions on practical diffractometry and crystal growth and selection were carried out.

Several participants brought their own samples, and a number of data sets were collected and solved throughout the workshop. Some participants also gave presentations on the final day.

Topics covered at the OpenLab Hong Kong:

1. Crystal Growth – Theory and Practice
2. Basics of X-ray Diffraction, Crystals and Symmetry
3. Structure Determination Overview
4. Selecting and Mounting Crystals
5. Diffractometer I. Pre-experiment: Unit-Cell and Space-Group Determination
6. Diffractometer II. Data Collection and Reduction
7. Using the *Olex2* Software Package
8. Structure Solution and Refinement

9. Validation, Tables and Figures
10. Databases and Publication
11. Special Topics

In addition, Michele Zema gave an introduction to IYCr2014 and a brief history of the IUCr. Special topics included the latest on refinement methods using invarioms given by Birger Dittrich and a lecture on neutron diffraction methods by Alison Edwards. All lecturers kindly made their lecture materials available for participants to continue to use after the workshop had finished.



Participants at the workshop dinner at Shatin Star Seafood Restaurant on Dec. 6, 2014. Photo credit: Herman Sung.

The overseas participants were housed on-campus along with the conference lecturers. Lunches and coffee/tea breaks were provided. A break was given to participants on the Friday afternoon, though many used the opportunity to carry out further lab work.

The OpenLab can be regarded as a success, with the goal of including a number of participants from the south-east Asian region. In particular it was pleasing that six participants from the Philippines attended, from five different universities, with the assistance of small travel bursaries of US$200 per person. Some follow up of progress made at the workshop should be forthcoming in 2015, with the suggestion of one or two crystallographic speakers and a possible one-day symposium at the upcoming Philippine

Chemistry Congress in April 2015. Contact should be maintained with Valerio de Grano of U. Santo Tomas to enable this future activity.

There is also the likely possibility of holding a future OpenLab in the area, either in Hong Kong or nearby, if some sponsorship money can be found. The total budget for the workshop was around US$15,000, including food, accommodation, travel money for independent lecturers and some travel bursaries. The total sponsorship money of US$10,000 from the IUCr-Agilent is gratefully acknowledged and was augmented by around US$5,000 from HKUST garnered in part from a previous Asian Crystallographic Association conference held at HKUST in December 2013. The venue for the workshop, which included a lecture theatre, separate classroom and access to chemical and X-ray diffraction laboratories, was supplied at no cost by HKUST.

Ian D. Williams, Chair, and Michele Zema, IUCr Representative

MEETING REPORT

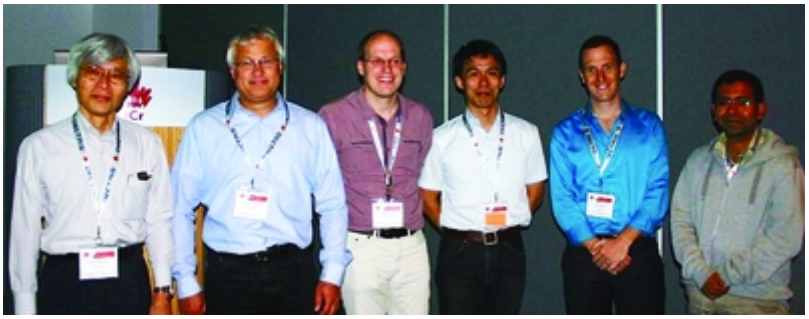
XXIII IUCr Congress and General Assembly

Continued from Volume 22, Number 3

The third and final part is in Volume 23, Number 1

Biological macromolecules

Macromolecular and soft-matter aperiodic crystals



MS57 speakers. From left: Y. Matsushita, S. Föster, M. Engel, S. Yakamoto, K. Barkan, V. Raghuwanshi.

The quest for 'soft-matter quasicrystals' (QCs) is an integral part of quasicrystal research. Macromolecular and soft matter aperiodic crystals were the topic of microsym. MS57. S. Föster (Germany), who found 18-fold symmetry for the first time, presented X-ray scattering data of block-copolymer micelles combined with new molecular dynamic simulation results of a Witten-Pincus model potential having two length scales. He also described new micellar and microgel QC systems. Y. Matsushita (Japan) talked about complex polymer melts and showed exotic morphologies, one of which was an approximant of the decagonal phase. Progress concerning theoretical and computational work was given by K. Barkan (Oregon) who extended their mean-field theory and showed cluster liquid QCs. M. Engle (USA) successfully stimulated a single atom (tetrahedrally-bonded) icosahedral QC using a two-length scale potential, considered to be the Holy Grail in this field for 30 years. Y. Sakamoto (Japan) described mesoporous silica QCs as polyhedral packing with relation to the Frank-Casper phases, and showed a large-scale QC made of binary silica spheres.

Tomonari Dotera

Ultimate resolution and neutron crystallography



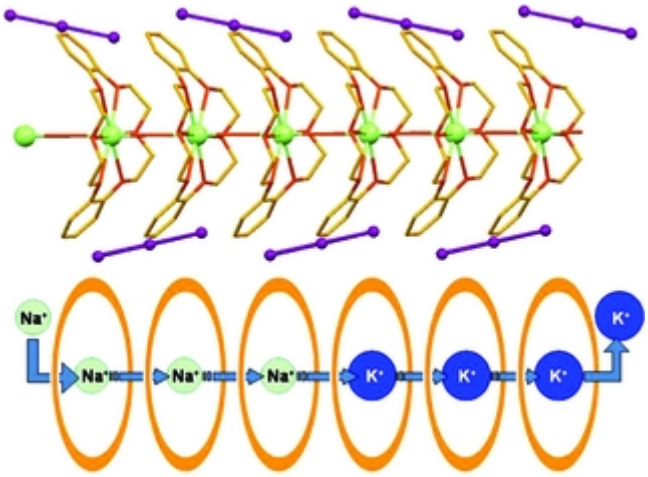
MS82 speakers and co-chairs. From left: Andrey Kovalevsky, Nobuo Niimura, Yu Hirano, Alberto Podjarny, Matthew Blakeley and Svetlana Antonyuk.

Microsym. MS82 focused on the information that can be derived from ultra-high resolution X-ray diffraction data (*i.e.* to 0.8Å or better) and neutron diffraction data extending to 2.5Å resolution or better. Z. Dauter (USA), Y. Hirano (Japan) and J. Kallio (Germany) illustrated the fine details revealed by ultra-high resolution X-ray studies, including the location of H atoms, bonding electrons, lone-pair electrons and multiple conformations. A. Podjarny (France), N. Niimura (Japan) and A. Kovalevsky (USA) described neutron crystallographic studies and showed that, despite the lower resolutions attained using neutrons, H atoms - including those that are relatively mobile - can be visualized, allowing the determination of protonation states and revealing details of hydrogen bonding and water structure that are important for a complete understanding of macromolecular function. The speakers emphasized the complementarity of X-rays and neutron studies. Y. Hirano (Japan) showed X-ray and neutron data for an 8.8kDa protein at ultra-high resolution, including detailed information for H atoms and some outer electrons.

Matthew Blakeley and Svetlana Antonyuk

Chemical crystallography

Supramolecular interactions in the solid state



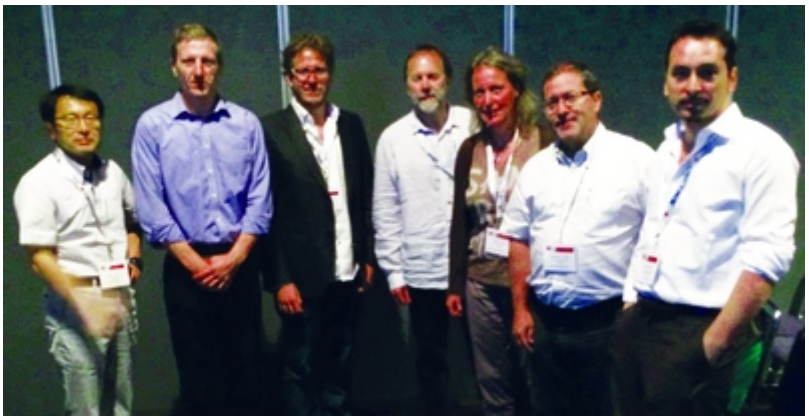
Alkali cation exchange and transport through supramolecular polyhalide-induced stacks of crown ether molecules. (Courtesy of Katharina Fromm.)

The wide scope of microsym. MS43 covered the preparation and characterization of supramolecular systems. G. Resnati (Italy) reported the formation of supramolecular gels *via* cooperative halogen and

hydrogen bonds. E. Boldyreva (Russia) presented variable temperature and pressure studies of continuous lattice strain, phase transition and crystallization. H. Uekusa (Japan) spoke about dynamic covalent bond formation and self-assembly in macrocyclic boronic esters. T. Mak (China) gave an overview of the *in situ* generation of silver-ethynide supramolecular synthons for high-nuclearity clusters. S. Chong (UK) described the study of purely organic molecular cage materials with significant porosity lacking strong directional interactions. K. Fromm (Switzerland) impressed the auditorium with 'supramolecular straws', compounds of DB18C6 macrocycle molecules, to form one-dimensional channels *via* halogen-halogen bonds using trihalides I_3^-, BrI_2^- and $BrIBr^-$ as anionic pillars. Potassium ions and water molecules are found inside three channel types, making ion transport possible. Using a single crystal as bridge between two compartments, one of which contains 1*M* NaOH and the other ultrapure water, the Fromm group was able to determine the kinetics at different temperatures by measuring the increase in ionic conductivity in the water compartment. The activation energy for Na^+ and K^+ transport through the channels corresponds to super-ionic conductors.

Petra Bombicz and Masaki Kawano

The role of crystallography in chemical reactivity and catalysis

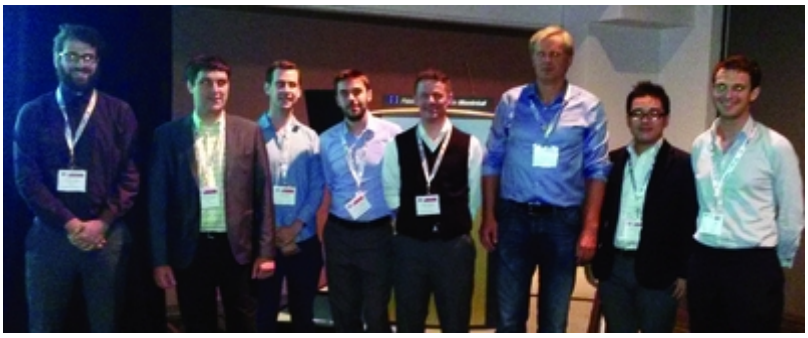


MS59 speakers and chairs. From left: Masaki Kawano, Andrew Bond, Guillermo Mínguez Espallargas, Lee Brammer, Alessia Bacchi, Fernando Lahoz and Pance Naumov.

Microsym. MS59 was attended by over 150 participants who learned how crystals might be used as reaction flasks and how they react to external stimuli, and how they jump and dance. M. Kawano (South Korea) showed how to obtain metastable permanently porous metal-organic frameworks (MOFs) and use them to trap rare species such as S_3. Kawano described the challenge of using thermodynamic and kinetic control to obtain porous coordination networks. G. Mínguez Espallargas (Spain) explained that in stimuli-responsive dynamic MOFs it is possible to switch magnetic properties on and off by modifying the content of dynamic pores. They explored how physisorption of different gases such as CO_2 or N_2 modifies spin and temperature transitions. A. Bond (Denmark) followed the kinetics of hydration and dehydration of sodium naproxen as a function of relative humidity, showing that complete crystallographic knowledge is crucial for pharmaceutical applications; a series of elegant synchrotron powder diffraction experiments followed the dehydration processes in approximately real time. J. Popovic (Croatia) was able to obtain heterobimetallic polymeric precursors of nanocrystalline mixed metal-oxide phases. L. Brammer (UK) showed that silver-based coordination polymers may mimic the supramolecular arrangement of carboxylic acids and can be so flexible as to rearrange their structures to accommodate small guests in latent pores, which are formed on demand. Finally, P. Naumov (UK) explained how crystals might literally jump by reacting to a change in temperature: this thermosalient effect converts packing energy into mechanical energy and it is strictly related to changes in the structure upon heating. The discussions that followed the talks generally pointed out that crystallography is the central science to define properties and applications of solid materials in all fields of modern technology, from catalysis to magnetic materials and from pharmaceutical science to mechanical engineering.

Alessia Bacchi and Fernando Lahoz

Experimental and simulated structures in metal-organic frameworks (MOFs)



MS75 speakers and chairs. From left: Ben Gelfrand, Francois-Xavier Coudert, Mathew Cliffe, Felipé Gandara, Stephen Moggach, Igor Djerd, Shuhei Furukawa and Thomas Bennett.
Microsym. MS75 focused on MOF structure solution and understanding the physical properties of these hybrid materials. B. Gelfand (Canada) is designing humidity-dependent proton conductivity in phosphonate-containing MOFs. S. Furukawa (Japan) focused on the surfaces of soft porous frameworks that can be modified to produce desired properties. Complex 'multi-layer' MOFs, consisting of a framework shell surrounding a different chemical interior, are multi-functional. Such materials can resist single-crystal formation, and I. Djerdj (Croatia) used powder diffraction to determine the structures of vanadium-based compounds. M. Cliffe (UK) examined disorder using pair distribution function analysis to probe the presence and interaction of defects in the structure of Hf-UiO-66. F. X. Coudert (France) developed a methodology to evaluate the flexibility of MOF structures and S. Moggach (UK) described the high-pressure behavior of extremely flexible scandium MOFs.

Thomas Douglas Bennett and Felipe Gándara

Crystallographic education

Crystallography education and training in the 21st century: new pedagogies, new paradigms, Part II



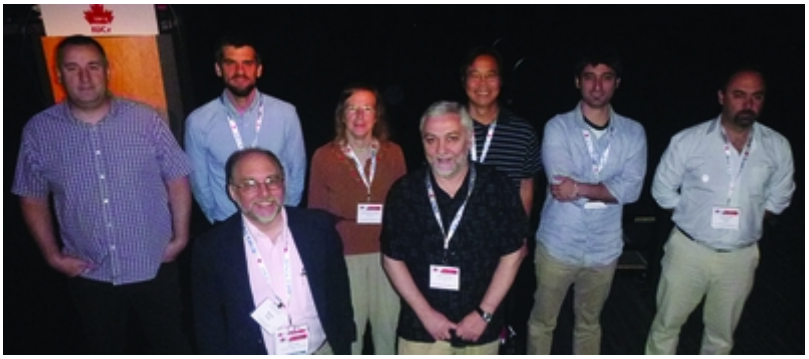
MS92 speakers and chairs. From left: Louise Dawe, Joe Tanski, Peter Moeck, Graciela Diaz de Delgado, Amy Sarjeant and Saulius Grazulis. Not pictured are Elena Boldryeva and Wael Rabeh.
Microsym. MS92 concerned educational approaches from around the world. P. Moeck (USA) described his efforts to generate 3D-printed models of crystal structures from coordinate files and to work with the Crystallography Open Database. G. Diaz de Delgado (Venezuela) spoke about the rich crystallographic heritage of Latin America; workshops held there, books and teaching materials developed in Mexico, and the 1974 Direct Methods School in Brazil. E. Boldryeva (Russia) described outreach programs for school children, including French language students who were inspired to pursue careers in science after

translating the French posters *Voyage dans le Crystal* into Russian. J. Tanski (USA), W. Rabeh (USA, UAE) and L. Dawe (Canada) described their methods to incorporate crystallography into undergraduate curricula, through laboratory experimentation or topical research and presentations.

Saulius Gražulis and Amy Sarjeant

Instrumentation, techniques and/or computation

Remote controls for crystallography at synchrotron and neutron sources



MS52 speakers and chairs. From left: (front row) Brian Toby and Ruslan Sanishvili; (back row) Dave Hall, Matt Suchomel, Marian Szebenyi, Craig Ogata, Daniele de Sanctis and Jean-Luc Ferrer.

While the benefits of remote operations are numerous, ranging from the simple conveniences of the home lab to significant travel-related financial, time and effort savings, they only work well if the functionality is not compromised for users, either by availability of tools normally offered at a beamline, or by cybersecurity and other restrictions. Effective communication between the on-site and remote components of the operation is also crucial. In microsym. MS52, the talks of C. Ogata (USA), D. Hall (UK), D. de Sanctis (France), M. Szebenyi (USA), J. Ferrer (USA) and M. Suchomel illustrated these points very well.

What became clear in this session was how far robotic systems for data collection have advanced. What seemed unthinkable just a few years ago, namely completely roboticized and automated handling of macromolecular crystals that are sensitive to mechanical impact, temperature, humidity and/or chemical environmental changes, now seems achievable.

The organizers could not locate any remote operation examples conducted at neutron sources. These instruments are often simpler than those found at synchrotrons and have very similar cybersecurity requirements. It is clear that such facilities will provide even greater benefit from remote operations, due to site-access restrictions and the longer data collection times. This is clearly a challenge for the future.

Ruslan Sanishvili and Brian Toby

Grazing-incidence surface techniques

Dramatic advances in grazing-incidence surface analysis techniques have accompanied technical advances in X-ray neutron scattering. Recent advances including *in situ* studies were presented in this symposium. In microsym. MS56, grazing-incidence small-angle X-ray scattering studies of sample preparation by spray coating and post-production treatments such as solvent-vapor annealing demonstrated the potential of accessing temporal changes on surface nanostructures. Kinetic processes monitored with time resolution down to tens of milliseconds allowed for understanding complex non-equilibrium processes. Neutron scattering techniques are able to study difficult sample environments, such as hot and wet surroundings. Sample modifications induced by these environments were analyzed in detail. Using the transmitted signal in grazing-incidence geometry was discussed.

Peter Müller-Buschbaum

Simultaneous methods with SAS



MS71 speakers and chairs. From left: (front row) Manfred Burghammer, Kohji Tashiro, Sylvio Haas, Satoshi Koizumi, Aldo Craievich, Bo Iversen; (back row) F. Zhang, Wim Bras.

The subject of microsym. MS71 was the on-line combination of small-angle scattering with other experimental techniques. K. Tashiro (Japan) described combining Fourier transform infrared spectroscopy with SAXS from synchrotron and conventional sources. S. Haas (Germany) demonstrated co-analysis of data sets obtained with SAXS and other techniques. This new methodological development has the promise to reveal correlations in chemical and structural events, which would remain hidden when using a sequential analysis of the data. B. Iversen (Texas) used the combination of SAXS with pair distribution function analysis in studies on the growth of nanocrystals.

Satoshi Koizumi and Wim Bras

In operando and structure evolution - from atomic to micron

The speakers in microsym. MS79 addressed the study of materials used in construction, catalysis, gas purification, energy storage and nanotechnology under operating conditions. The structural changes during the simultaneous sorption of different gases by porous materials and the structural changes of new iron-based electrodes used in batteries are being characterized using wide-angle neutron diffraction. The switching process of thin films of thermoresponsive polymers is followed using time-resolved time-of-flight neutron reflectometry. The formation of metal layers on nanostructured polymer templates is investigated during the sputtering process. New instruments are being developed, such as the neutron diffractometers iMATERIA and SPICA at J-PARC, dedicated to the study of industrial materials and to *in situ* investigations of battery materials, respectively. Specialized sample environments, *e.g.* humidity chambers for neutron reflectometry and gas sorption systems, and sensitive methods, such as phase-sensitive and modulated enhanced X-ray powder diffraction, are becoming available.

Christine Papadakis and Vanessa Peterson

Materials or minerals

Symmetry and isomorphism in material design and crystal growth



MS62 speakers and chairs. From left: J. Huot, R. Kozak, E. Vlieg, L. Suescun, T. Bekker, R. Černý, A Dąbkowski.

Crystal growth is a complex process, which classically can be described by thermodynamics and heat- and mass-transport terms. However, this approach cannot explain numerous observations - facets, crystal growth anisotropy, isomorphism (and isomorphic substitution), to name just a few. Knowing the crystallographic structure is necessary to fully understand the crystal growth process and to utilize isomorphic effects in synthetic procedures. The speakers in microsym. MS62 addressed these topics.

E. Vlieg (The Netherlands) told us about the breaking of symmetry in compound crystallization, an important problem in the synthesis of organic and inorganic materials. He also addressed effects of symmetry breaking on the crystal surface - an issue important to microscopic understanding of crystal growth and nucleation. R. Černý (Switzerland) introduced us to the peculiar properties of borohydride anions that are capable of forming metal borohydrides, which resemble metal oxides.

T. Bekker and A. Dąbkowski

Recent development of wide band gap materials: semiconductors and oxides



MS94 speakers and chairs. From left: M. Lorenz, S. Pimputkar, S. Garcia-Granda, D. Klimm, E. Bøjesen, T. Oshima, S. Harada.

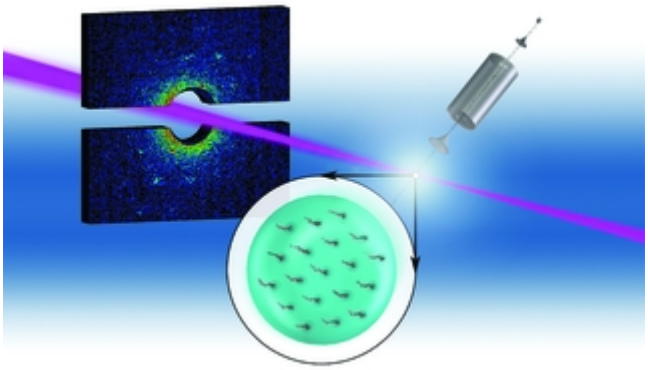
The papers by Teal *et al.* in *Phys. Rev.* (1950, 1951) marked the introduction of semiconductors into technology. Soon germanium was replaced by silicon, which is still the material of choice for most electronic devices. For some applications, such as optoelectronics in the visible or even ultraviolet spectral range, or for high-power electronics, 'wide band gap' semiconductors are needed, where the energy difference between the valence and conduction bands is considerably larger than for Si. In this

session, the status of wide band gap research and application was reviewed. In microsym. MS94, talks by S. Harada (Japan) and S. Pimputkar (USA) were devoted to SiC or GaN, respectively. Both substances have already been introduced into commercial applications such as solid-state lighting, but nevertheless the improvement of bulk growth processes with respect to size, quality and cost efficiency is still an issue, and the application of crystallographic analysis methods has afforded remarkable technological progress. The other four talks were mainly devoted to semiconducting oxides, with focus on ZnO by L. Leipzig (Germany) and E. Bøjesen (Germany), CdS by G. Granda (Florida), and b-Ga_2O_3 by Oshima (Japan) in nanostructures and layers, as well as in the bulk. Impressive results were presented, ranging from *in situ* diffraction studies on phase formation during the growth of ZnO nanocrystals to oxide-based devices such as ZnO transistors or Ga_2O_3 based solar blind UV light detectors.

D. Klimm

Physical and/or fundamental

Advances in X-ray FEL coherent scattering and diffraction



Single-shot X-ray coherent diffractive imaging experiment detects lattices of quantum vortices in rotating superfluid helium nanodroplets. (Courtesy of Oliver Gessner.)

Short-wavelength free-electron lasers (FELs) have been in operation since 2005. The first facility to provide this radiation was FLASH in Hamburg, operating in the XUV range. Ultra-short pulse duration, nearly complete transverse spatial coherence and very high pulse intensities provided the basis for new X-ray applications and scientific insight. Since 2010 the LCLS at SLAC, and since 2011 SACLA at SPring-8, also provide hard X-ray FEL radiation. Microsym. MS20 provided an overview of the recent advances of hard X-ray FEL coherent scattering and diffraction experiments, and their application to materials science, quantum systems and structural biology. The characterization of FEL coherence properties and the possibility to simulate complete FEL coherence experiments were discussed. All discussed applications used single particles to be studied, either mounted on a thin membrane or injected into the FEL beam. These single particles are, however, very different and include gold nanocrystals, Xe-doped He droplets, frozen hydrated cells mounted on Si_3N_4 (or C) membranes or free-flying bio-particles. Particularly stunning were the results obtained by coherent diffraction imaging at the LCLS from cryogenic ^{4}He droplets. O. Gessner (LNBL) showed how it was possible, using this technique, to observe the existence of a vortex lattice with contrast enhancement by Xe doping and to measure the deformation of the droplets due to very high precession frequencies, and how these results contribute to determining the superfluidic state of the droplets.

Another very important talk presented the status of single biomolecule imaging using X-ray FEL radiation. S. Boutet (SLAC) showed the present status of experiments and explained the instrumentation developments in the areas of X-ray delivery, background suppression and sample injection still to be achieved, to bring this technique to fruition.

Changyong Song and Thomas Tschentscher

Methods: algorithms and software for powder diffraction



MS72 speakers and chairs. From left: Yifeng Yun, Reinhard Neder, Takashi Ida, Xim Bokhimi, Ryoko Oishi-Tomiyasu, Tsunehisa Kimura.

While powder diffraction methods are well established, there are still challenges for difficult samples. In microsym. MS72, R. Neder (Germany) examined the effects of preferred orientation on the pair distribution function (PDF). The Debye equation implies a spherical averaging and this assumption is invalidated by preferred orientation. The computational demands for such calculations are high. Computational methods were a theme of the session. X. Bokhimi (Mexico) described how CPU technology is powerful enough to fully ray-trace a diffractometer, and O. Oishi-Tomiyasu (Japan) demonstrated how mathematical methods have impacted powder indexing. Even 'grainy' samples can now lead to reasonable structural refinements, due to the statistical methods described by T. Ida (Japan).

Y. Yun (Sweden) described how electron diffraction could be used to solve structures in a multi-phase system. T. Kimura (Japan) showed how preferred orientation might be induced in a suspended sample by applying a magnetic field. By measuring 2D diffraction data from a magnetically oriented sample the crystal symmetry may be deduced.

Jon Wright

Frustration, topology and chirality in metals and complex oxides



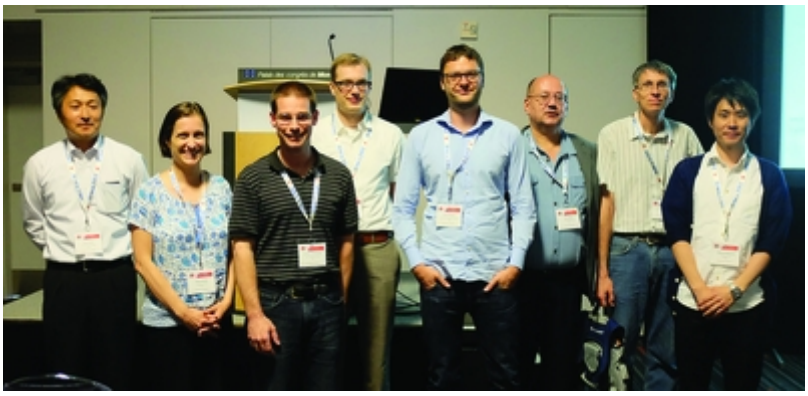
MS105 speakers and chairs.

The issues discussed in microsym. MS105 were related to frustration, topology and chirality of magnetic intermetallic or oxide compounds. The topics ranged from rather long-standing ones, such as frustrated and quantum magnets, to modern ones, including topological insulators and chiral skyrmion magnets.

Of particular note was a talk by J. Paddison (UK) who demonstrated that powder magnetic diffraction data could be used to retrieve the short-range spin correlations in crystalline frustrated magnets. He showed that even hidden multiple orders might be detected in gadolinium gallium garnet using this analysis method. This suggests a promising future of this approach for frustrated magnetism research.

Taku J. Sato

Surfaces



MS111 speakers and chairs. From left: Yuki Fukaya, Joanne Stubbs, Christian Schlepuetz, Jim Ciston, Daniel Schwarz, Peter Moeck, Craig Bennett, Tetsuroh Shirasawa.

Microsym. MS111 highlighted probes ranging from charged particles (electrons and positrons) to scanning probe microscopies to X-rays. Attendees were introduced to total-reflection high-energy positron diffraction (TRHEPD), which 'sees' only the uppermost 1-3 layers of atoms on a surface, by Y. Fukaya (Japan), and saw examples of three-dimensional X-ray reciprocal space maps that allow for the discovery and exploration of unanticipated diffraction features, enabling the description of complex symmetries and structures in thin films, presented by C. Schlepuetz (USA). The use of polychromatic X-rays to collect rapid crystal truncation rod (CTR) data demonstrated this oft-used but usually slow technique could also be suitable for time-resolved studies by T. Shirosawa (Japan). We saw that scientific movies (made with low-energy electron microscopy or LEEM) not only illustrate and entertain, but can also be used to quantitatively describe surface nucleation rates and adsorbate structures by D. Schwarz (USA). A new approach to image processing based on plane group symmetry provoked a thoughtful reexamination of traditional STM image analysis and interpretation by P. Moek (USA), and a new description of charge-density waves in $NbSe_3$ by T. Bennett (UK) helps to resolve discrepancies in a variety of previously published data. Taken together, all of these methods provide exciting new opportunities for understanding crystallographic aspects of surfaces, interfaces and thin films.

Joanne Stubbs and Jim Ciston

IUCR ACTIVITIES

Report from Executive Committee

General Assembly



Back row: M. J. Cooper (Convener, IUCr Finance Committee), M. H. Dacombe (Executive Secretary). Executive Committee: J. M. Guss, R. Kuzel, M. Takata, W. Depmeier and S. Garcia-Granda. Front row: H. Dabkowska, L. Van Meervelt (General Secretary and Treasurer), M. L. Hackert (President), A. M. Glazer (Vice-President) and G. R. Desiraju (Immediate Past President).

The General Assembly held three sessions at the Montreal Congress. Applications for membership from Costa Rica, Pakistan, Turkey, Uruguay, Venezuela, Morocco, Cameroon and Algeria were accepted (all in Category I). The Minutes of the Twenty-Second General Assembly in 2011 were approved, and the triennial financial report and the reports of the Executive Committee, the Commissions, the Scientific Associates and Regional Associates and the Union Representatives on Other Bodies since the Twenty-Second General Assembly in 2011 were accepted. The excellent success of the International Year of Crystallography was noted. New officers of the Union, Chairs and members of Commissions and Union Representatives were elected and the appointments of Editors of the Union were confirmed. The formation of a new Commission on NMR Crystallography and Related Methods was approved (see article here). The Commission on Synchrotron Radiation was re-named the Commission on Synchrotron and XFEL Radiation, and the Commission on Crystallography of Materials would continue with *ad interim* status. The recently formed Latin-American Crystallographic Association (LACA) was accepted as a Regional Associate. The Reports of the Chair of the Sub-committee on the Union Calendar, the Chair of the Committee for the Maintenance of the CIF Standard, the Chair of the Diffraction Data Deposition Working Group and of the Editor of the IUCr Newsletter were received. The good progress of the IUCr/Oxford University Press Book Series was noted. The General Assembly approved the recommendation that the unit contribution should remain unchanged at CHF 1,000 for the years 2015–2017 inclusive. Progress with plans for the Twenty-Fourth General Assembly in Hyderabad, India, were noted and the General Assembly accepted an invitation to hold the Twenty-Fifth General Assembly and Congress in Prague, Czech Republic, in 2020.

Executive Committee

The Executive Committee met for several days before and most days during the Congress, mainly to deal with matters directly related to the business of the General Assembly and the work of the Commissions. Particular emphasis was placed on the development of the IUCr journals, new Volumes for International Tables, all aspects of the International Year of Crystallography, and the work of the Sub-committee on the Union Calendar. The OpenLabs were proving a great success and promising initiatives resulting from the three summit meetings were anticipated. Following the General Assembly sessions, at the joint meeting of old and new Executive Committees it was decided that written instructions on the conduct of elections within Commissions (when preparing recommendations for membership) and guidelines for countries applying for membership of the Union would be prepared. It was agreed that it

was important to ensure the legacy of the International Year of Crystallography so that the many initiatives that had proved successful could be maintained. An IYCr legacy Fund was established.

Michael Dacombe

MEETING REPORT

Crystallographic Society of Japan

Tokyo, Japan, November 2014
www.crsj.jp/activity/annualMeetings/nenkai2014/



The winners of the 2014 CrSJ Awards with the President of CrSJ (from left): Nishimasu, Tanaka, Miki (President), Senda and Fujii.



The poster Awardees and the President of CrSJ (from left): Tomita, Kawai, Morita, Miki (President), Komatsu, Hibino and Kanaya.

Over 423 crystallographers participated in the 2014 annual meeting and the general assembly of CrSJ held at the U. of Tokyo, 1-3 November. The meeting featured 49 oral and 165 poster presentations covering all aspects of crystallography, four award lectures, three microsymposia (a total of 14 invited talks), a CCP4 workshop, a special lecture promoting gender equality, five luncheon seminars, industrial exhibitions from 15 companies/organizations and a special symposium celebrating IYCr2014.

The IYCr commemorating symposium was held in the morning of 2 November, where leading scientists from various research fields presented lectures: 'Oxide electronics and crystals' by M. Kawasaki (U. Tokyo), 'Super conducting under extreme conditions and crystals' by K. Shimizu (Osaka U.), 'Protonics

and crystals' by H. Kitagawa (Kyoto U.) and 'Energy generation and crystals' by N. Kamiya (Osaka City U.).

At the CrSJ Awards Ceremony, the S. Nishikawa Award was presented to I. Tanaka (Hokkaido U.), the Research Award was given to T. Senda (KEK), and the Young Crystallographer Awards went to H. Nishimasu (U. Tokyo) and K. Fujii (Tokyo Inst. Tech.).

Six young scientists were honored with Poster Awards. They are A. Tomita (KEK), H. Kawai (Osaka U.), J. Morita (U. Tokyo), Y. Komatsu (U. Hyogo), K. Hibino (Tokyo Inst. Tech.) and H. Kanaya (Osaka Pref. U.).

A full program of the meeting can be viewed at the CrSJ website http://www.crsj.jp/activity/annualMeetings/nenkai2014/. The chair of the organization committee was M. Tanokura (U. Tokyo) and the program committee was chaired by K. Ogawa (U. Tokyo).

Tomoji Ozeki

MEETING REPORT

Heart of Europe Bio-Crystallography

Berlin, Germany, September 2014
www.helmholtz-berlin.de/events/hec/



Participants at the 17th Heart of Europe bio-Crystallography meeting in Berlin, Germany.

The annual event of the middle European community of macromolecular crystallographers, the HEC-17 meeting, was organized by the Macromolecular crystallography group, Helmholtz Zentrum Berlin, in the Akademie Schmöckwitz in Berlin at the end of September. Traditionally, the conference is focused on presentations of young biological crystallographers from a number of German, Polish, Czech and Austrian research groups. The event has become one of the most important and inspiring opportunities for young researchers in the field to both present their own results to an audience with similar focus and maturity level and at the same time take the advantage of learning basic or advanced approaches from their colleagues. This year the HEC organizers created a warm and welcoming environment and provided excellent technical and organization support throughout the three-day conference. All the 132 participants enjoyed the 31 scientific presentations, mostly from students of some 27 research groups around middle Europe. The HEC lecture, usually given by a prominent scientist from outside the HEC community, was presented by Prof. Gerhard Klebe, University of Marburg, entitled 'Fragment-based Lead Discovery: An Efficient Alternative in Structure-based Drug Design'.

Every year the HEC prize is awarded to the young scientist presenting the best talk of the conference. The panel of six judges had a difficult decision to make as a large number of presentations reached the highest ranks. The 2014 HEC prize was awarded to Asgar-Abbas Karzani (IIMCB Warsaw) for his very enthusiastic lecture 'Crystal structure of 5hmC specific endonuclease PvuRts1'.

All conference participants could take part in the main social event of the second day of the conference – the Dragon boat race. Six teams of thirteen (12 rowers and 1 drummer) were drawn, and after 30 minutes of training the race began, in groups of three boats. The finals saw a fierce fight and only small finish line differences of tens of centimetres decided the golden team – the team 'SCHATZI' led by Karine dos Santos from the FU Berlin. The HEC 17 conference was supported by a number of sponsors which contributed to the high level of the event and to the fine facilities for the nearly 100 young scientist participants.

The HEC prize was supported by the IUCr. The HEC bio-crystallography community was invited to the next meeting to be organized by the Czech Society for Structural Biology in Kutná Hora, Czech Republic, 24-26 September, 2015.

Jan Dohnálek

IUCR ACTIVITIES

New IUCr Commission on NMR Crystallography and Related Methods



9.4 T wide-bore magnet used in an NMR spectrometer for work on solids (proton resonance at 400 MHz).

As a result of a submission to the IUCr meeting in Montreal last August (2014), a new Commission has been established to cover magnetic resonance methods of studying crystallography. Actually, although in a sense new to IUCr, NMR has been known as a method of obtaining detailed molecular-level information on crystalline materials for about 60 years. For instance, in 1948 (only three years after the discovery of the NMR phenomenon) Pake reported the measurement of the internuclear distance between protons in water molecules involved in gypsum. A year later, Gutowsky et al. commented that 'the development of experimental methods for observing nuclear magnetism has provided a means of investigating certain aspects of molecular and crystal structure'. However, much higher resolution was attainable for solutions than for solids, so for several decades, the former dominated NMR work and the latter languished. This situation changed with the development of cross polarization, magic-angle spinning and high-power proton decoupling in the mid 1970s. This combination of techniques resulted in much higher resolution for solids, so that applications to crystalline materials have become common. The crystallography community in general has been slow to adopt NMR as one of its key techniques, so NMR and diffraction methods have largely involved separate communities until recently. However, it has become obvious that the complementarity of these methods requires a closer interaction of their practitioners, so the formation of a new IUCr commission at this point makes sense. The development of computational methods for refining structures from NMR data has added urgency to this matter.



Participants in the fourth SMARTER meeting.

The requirement for closer integration of NMR with other methods of studying crystalline materials was highlighted by a short article in the *IUCr Newsletter* in 2005, following an International School on Crystallography at Erice the previous year, which had included lectures on NMR. It should be noted that the Commission will also deal with other magnetic resonance techniques, such as ESR/EPR.

It is worth summarizing here just a few of the salient points about NMR crystallography for the benefit of newcomers to the subject:

- NMR is generally used to study microcrystalline samples and does not require single crystals.
- It gives information about short-range environments of atoms in a complementary fashion to diffraction techniques, which rely on long-range order.
- Motion in solids can be monitored and investigated.
- Crystallographic disorder can be detected and evaluated.
- Amorphous systems yield detailed information about molecular-level structure.
- The structure of heterogeneous materials can also be evaluated by NMR.
- Since the technique is based on nuclei not electron density, the correct positions of hydrogens are relevant.
- It can be used in combination with powder diffraction (and even, in some circumstance, on its own) to obtain full structural information.

The sheer versatility of NMR should also be emphasised. This arises from (*a*) the fact that nearly all the elements of the Periodic Table have a suitable isotope for study (and the frequency ranges for their signals do not, in general, overlap) and (*b*) there is a wide variety of experiments which can be performed by varying the radiofrequency pulse sequences used. Further details can be seen in a number of books. There is, for example, a recent (2009) handbook on 'NMR Crystallography' (ISBN 978-0-470-69961-4). A series of 'SMARTER' conferences has been instituted on this topic, the fourth being held in Durham (UK) in September 2014; these are now sponsored (*inter alia*) by IUCr.

The new Commission is chaired by Francis Taulelle (France), with joint secretaries Robin Harris (UK) and Manish Mehta (USA). Other current members are Tatyana Polenova (USA), Marek Potrzebowski (Poland) and Rod Wasylishen (Canada), with IUCr consultants Gautam Desiraju (India) and João Rocha (Portugal). Further members are to be added. Details of the objectives and activities of the commission can be found on the IUCr web site under www.iucr.org/iucr/commissions/nmr-crystallography. Comments and queries about the plans of the Commission can be addressed to r.k.harris@durham.ac.uk or mmehta@oberlin.edu.

Francis Taulelle, Manish Mehta and Robin Harris

REGIONAL NEWS

ACA History Website Adds 'ACA Beginnings'



Martin Buerger



Elizabeth Wood



William Parrish

ACA Historian Virginia Pett and webmaster Patti Potter have inaugurated a new section to the ACA History website. 'ACA Beginnings' will contain articles and photographs documenting the history of the organization and the people who have made it a vital forum for scientists interested in structure and the significance of structure for understanding mechanism and function. See www.amercrystalassn.org/history_beginnings.

The first item in this new section is the text of a 1974 talk by Martin Buerger relating how the ACA was formed in 1950. Buerger was the inventor of the precession camera and the author of many books describing fundamentals of crystallography and how to obtain undistorted photographs of the reciprocal lattice. He was president of both the American Society for X-ray and Electron Diffraction (ASXRED) and the Crystallographic Society of America (CSA), the two precursor organizations that united to form the ACA in 1950.

A second article by Elizabeth Wood and William Parrish describes the formation of the ACA and some of the 'culture' of the new group: the friendliness and the sense of humor that pervaded the meetings as well as the informal style of an organization with no headquarters and no regular publication in the early days.

Virginia Pett

AWARDS AND PRIZES

PANalytical Award supports young scientists

PANalytical is one of the world's leading suppliers of analytical X-ray instrumentation and software. The company seeks to reward early-career scientists who have demonstrated innovative thought to their research when using an X-ray analytical technique with a $5,000 prize. The Award in 2012 went to Thomas Bennett (UK). Ana Cuesta (Spain) received the 2013 Award for her investigation of yeelimite, the most important phase in calcium sulfoaluminate cements.

The winner of the 2014 Award will be decided in early 2015 by a selection committee that includes established research scientists unaffiliated to PANalytical. Submissions for the 2015 Award will be possible from June 1, 2015 with a deadline of December 1, 2015 (www.panalytical.com/award). Applicants must publish a paper during the period 1 January 2014 – 1 December 2015 that demonstrates ground-breaking thinking in a topical field. There are no restrictions on the manufacturer of the X-ray equipment used. Questions can be addressed to award@panalytical.com.

NOTICE

ECM 2015

Rovinj, Croatia, 23-28 August 2015

http://ecm29.ecanews.org/

The 29th European Crystallographic Meeting will be held in Rovinj on the magnificent coast of Istria (Croatia), below the Lim Fjord. Its crowded houses, narrow streets and small squares are untouched by modern urbanism.

Rovinj is accessible from airports at Pula (40 kilometres from Rovinj), Zagreb (262 km from Rovinj), Ljubljana (205 km) and Trieste (147 km).

The sessions will be held at the AECC – ADRIS Exhibition and Convention Centre (an old tobacco factory that is an extraordinary example of the industrial architecture of the late 19th century). It is a few minutes' walk from a dozen hotels and the majestic old town.

The abstract submission deadline is 23 March 2015. Abstracts should be submitted *via* the website http://ecm29.ecanews.org/programme/abstract-submission/, where the guidelines for the online abstract submission will be available.

The presenting author must be registered at the conference by 23 May 2015 at the latest, in order for his or her abstract to be included in the programme book. One registered participant can be the presenting author of only one abstract. However, every participant can be a non-presenting co-author on any number of abstracts.

'Early bird' registration payments must reach the ECM29 account by 23 April 2015 at 11:59 PM, Zagreb time. The regular rate registration deadline is 23 May 2015, and the late registration rate applies after 23 May 2015.

A limited number of bursaries are available for PhD students and young scientists (under 35). An applicant for a bursary should be the presenting author of an abstract submitted *via* regular online abstract submission procedures by 23 March 2015. The following documents are also required: (1) Bursary application form, (2) Curriculum Vitae with list of publications, (3) Recommendation letter from Supervisor or Head of the Department/Group. The letter should confirm the status of an applicant (PhD student, post-doc etc.). Only applications containing all the required documentation will be considered for a bursary.

The bursary application form and accompanying documents should be sent by e-mail no later than 23 March 2015 to: Bursary Committee ECM29, e-mail: asantic@irb.hr

A decision about the bursary application will be communicated to all applicants by 7 April 2015. If your application is successful, the conference agent will contact you *via* e-mail regarding organising your registration account. Registrations made through the automated system and paid for will not be refunded, and your bursary application will be made void. After providing the necessary information, the agent will proceed to register you and organize your services according to the bursary agreement, and send you the appropriate documents for payment.

excerpted from BCA Crystallography News September 2014

NOTICE

Zurich School of Crystallography 2015

Zürich, Switzerland, 7-20 June, 2015

www.chem.uzh.ch/linden/zsc/

Time is running out to get your applications in to attend the ever popular Zürich School of Crystallography, to be held 7-20 June 2015 at the U. of Zürich, Switzerland. The school is ideally suited to young researchers in the molecular and solid-state sciences who do not have access to crystallographic courses at their own institution.

Participants will gain hands-on experience in the science and art of routine single-crystal and molecular structure determination of small molecules through lectures, computer exercises and practical work. During the School, students will have the unique opportunity to use an X-ray diffractometer to collect data and determine the structure of one of their own compounds that they are currently interested in.

Ten tutors experienced in all aspects of chemical crystallography will be on hand to teach the theoretical and practical aspects of this sometimes complex science, ensuring plenty of individual guidance throughout the School.

To find out more about the School and to apply please visit www.chem.uzh.ch/linden/zsc/.

Tony Linden and Hans-Beat Bürgi