Crystallography News

British Crystallographic Association

Issue No. 144 March 2018
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Spring Meeting in Warwick soon; Group Meetings held

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This month's cover:

Welcoming Warwick University scenes, relaxed BSG speakers, intense IG/CCG session

From the President

AT the time of publication of this issue of CN my 3-year term as BCA President will be coming to an end. I have enjoyed my involvement and have appreciated working with an excellent team of people who have been members of BCA Council during this time and particularly the ever-present BCA Officers, Richard Cooper, Claire Wilson and Pamela Williams, with whom I've worked most closely. I think the BCA remains in good health, both in terms of its meetings and its membership, but it will need the continued support not only of the membership as a whole, but particularly of volunteers who step forward to take on the roles within BCA Council, the groups, and the programme committee(s). These volunteers ensure that we can continue to have a BCA that reflects the broad interests of the community and continues to welcome new ideas, new techniques and new research that has an impact on structure across the scientific disciplines.

One aspect of becoming BCA President that I hadn't anticipated was that I would be handed a twitter account (thanks @d_a_keen). It's provided an interesting introduction for me to the world of twitter, with its combination of useful information, insights, humour and the bizarre, all of which have come across my path as a result. I'm certainly now of the view that it is valuable for the BCA to engage via twitter as one of its means of communication. I have had to make sure that I remember that the account is that the BCA President and not my account. You can follow the account @BritCryst_Pres, which will soon be handed over to the newly elected President.

As I write this column we are coming to the end of the voting period for elections to the new BCA Council. I am grateful to all the candidates who have been willing to stand for election. We will know the outcomes quite soon and can begin work on a smooth transition to take place at the Spring Meeting. I will report on the first cycle of this new election process at the AGM. I look forward to working with those elected in my back-seat role as Past President over the coming year.

The Spring Meeting in Warwick is now not far away and promises again to be an excellent line-up of symposia, speakers and poster presenters. I am grateful to Programme Chair **Leo Brady** and the whole Programme Committee for their commitment over the past year in putting the meeting programme together, and to our colleagues at Hg3 for again smoothly handling the logistical side of the conference planning and delivery. The main meeting will feature Awards lectures from **Bill Clegg**, who will give the *Lonsdale Lecture*, and **Eleanor Dodson**, who will give the *Dorothy Hodgkin Prize Lecture*. Wednesday afternoon will include the *Early Career Awards Symposium*, featuring lectures from the awardees of the BCA groups. The YCG satellite meeting, held directly prior to the main meeting, will feature the *Parkin Lecture*, delivered this year by **Michael Gaultois** of University of Cambridge.

Looking further ahead, the 2019 Spring Meeting will see us return to Nottingham, which provided an attractive venue in 2016. I'm pleased that **Emma McCabe** (University of Kent), has agreed to be Programme Chair for the 2019 meeting. Preliminary planning will begin, as in recent years, with a short meeting of programme committee members to be held on the final day of this years' Spring Meeting (Thursday March 29th).

I will close the column with the sad news of the recent death of Prof. **Terry Willis** (Oxford University) on January 18th. Terry was one of the pioneers in neutron scattering and crystallography and was central to establishing neutron diffraction at the Harwell site near Oxford. He is well known through his research, his books and the long-running summer schools on neutron scattering. He was a founding member of the BCA and awarded Honorary Membership in 1999. An extended obituary can be found on page 22 of this issue. He will be sadly missed.

Lee Brammer

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Full committee details on the BCA website

www.crystallography.org.uk

From the Editor

OUR Spring Meeting is rapidly approaching. The details in this issue and on the website should convince anyone who is still undecided that this is a meeting which simply cannot be missed. Our cover shows 3 scenes from the University of Warwick, starting with the Sciences Building, the venue for our scientific sessions. Before some previous Spring Meetings I promised you ducks; there are water features at Warwick that might attract them. I thank Amy Stares for the BSG Meeting pictures and Cheryl Doherty for the IG/CCG meeting picture.

Two other meetings should inspire you to put fingers to keyboard and dash off a couple of brilliant abstracts. (When I started in crystallography, I'd have said "put pen to paper". I suppose some of you will now put fingers to touchscreen. I still wince slightly when I do this, remembering how I used to tell off my students when they touched the screen of my precious Silicon Graphics workstation with greasy fingers.)

But I have digressed. The American Crystallographic Association meeting will take place from 20-24 July. For those of you who think that The Donald might not let you in, worry not! Because this year's venue is Toronto, you can expect a hearty Canadian welcome. Toronto is a beautiful city with a scenic lakefront and unspoiled country nearby. Important deadlines are March 30 for abstracts, May 31 for Early Bird registration and June 18 for reserving a discounted room at the conference hotel. The topic of this year's Transactions Symposium is "Shining a Light on Structure-Based Drug Design".

A month later we'll be able to enjoy the European Crystallographic Meeting in Oviedo, Spain. Dates to enter into your diary are 22-27 August for the actual meeting, 22 April for Early Bird registration and 29 April for abstracts. Being located in the extreme north of Spain at an altitude of 80 to 709 m above sea level, Oviedo escapes the searing Spanish summer heat. In August the average high at the weather station is 23.3°C. These conditions, along with a compact historic district and pleasant parks, make Oviedo a good place to enjoy a brisk walk before or after spending time in lectures. The European Union has named this city on a list of the cleanest cities in Europe.

With glacial slowness I have produced a write-up of *last year's* meeting of the German Crystallographic Society (DGK). The timing does have one advantage. The first plenary lecture was given by Prof. **Ilme Schlichting** on the subject of "Protein structure and dynamics using X-ray free electron lasers". My brief summary cannot possibly do justice to a fascinating lecture on the hottest of hot topics, but I hope it will whet your appetite for this year's BCA Spring Meeting, where the BSG plenary lecture will be given by none other than… Ilme Schlichting. As for this year's DGK meeting, you have just enough time to book last-minute travel tickets and pack your bag. While the 2017 meeting was held in late March, this year it moves forward to 5-8 March. Furthermore, while last year's venue was Karlsruhe in the balmy wine-growing southwest of Germany, this year it is Essen with its more bracing climate. The evolution of Essen is fascinating. It has gone from a powerhouse of heavy industry to rustbelt to a burgeoning new centre of culture and high tech. Last year it was selected as the European Green Capital.

Other meeting reports are featured in this issue too. In November 2017 our Industrial and Chemical Crystallography Groups joined forces for an Autumn Meeting on a topic, "Design of Crystalline Products" that was relevant to both groups. The presentations revealed cutting-edge research in the determination and prediction of crystal structures along with its great technological importance. Just a week before Christmas our Biological Structures Group held its Winter Meeting. Perhaps to blow away some excessively frothy Christmas cheer, they introduced a note of anguish as well as exultation with the title "The Joy and Pain of Structural Biology Research". Although the cover shows that they still had a good time, presentations by a stellar array of speakers demonstrated that the Latin motto "Per aspera ad astra" could well be applied to this area of research. Then the New Year got off to its customary mind-opening start in the form of the CCP4 Study Weekend in Nottingham. You may recall that the BCA contributed support for two participants to attend the 1st Pan African Conference of Crystallography in October 2016. Their reports in this issue show how much they benefited.

In this issue we have an obituary for **Terry Willis**, who did such important work in the development of neutron crystallography in the UK and promoted its use *via* collaboration with academic scientists including **Dorothy Hodgkin**. He also co-authored books which became classics and organised schools on neutron scattering. It is fitting that we pay tribute to his brilliance as a scientist and helpfulness to colleagues.

With sadness I read the death notice on the IUCr website for Professor **Alajos Kálmán**. He was a distinguished chemical crystallographer at the Hungarian Academy of Sciences, for whom ResearchGate lists 424 publications. I became acquainted with him through his important research on the structure of heterocyclic compounds, which matched interests of mine. Even while Hungary was ruled by communism, he always seemed ready to have a free-ranging scientific discussion. Those of you who have followed my presentations at recent BCA meetings will know that impossibly close H…H contacts in published structures are a concern of mine. Together with his colleagues **Petra Bombicz**, **Mátyás Czugler** and **Roland Tellgren**, in 2003 he published the structure with the then shortest known genuine C-H…H-C contact [1.949(7) Å], refcode TACRIB04, verified by neutron as well as X-ray diffraction. Perhaps we should be grateful for the isolation imposed by the Iron Curtain. This polymorph (A) of 1,2,3,5-tetra-O-acetyl-β-D-ribofuranose was the first one prepared, in 1947; but by 1964 laboratories in western Europe, the USA and Australia could only grow a more stable polymorph (B). However, in 1981 polymorph A reappeared in Budapest and was carefully protected from contamination since then. Its excessively short H…H contacts may well be the reason why it is a disappearing polymorph.

Carl Schwalbe

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Puzzle Corner

IF you have been watching **Brian Cox**'s *Forces of Nature*, you will have seen his illustration of hexagonal snowflakes forming from interacting water molecules, which are in no way hexagonal. Yet some symmetrical molecules form crystals that do not "use" their symmetry. Of the following molecules, which form(s) crystals with the highest symmetry: cyclobutane, cyclohexane, benzene or cubane?

Answers to December Puzzle Corner

THE 2018 European Crystallographic Meeting will take place in a very pleasant corner of Spain. From the following chemical or crystallographic clues derive symbols that give them a holiday message.

F E Main ingredient of steel
L I Its ions power highly energy-dense batteries
Z Number of formula units in the unit cell

N A Related to the element in the second clue; too much could give you high blood pressure
V Transition metal next to titanium
I Represents a body-centred cell
D Big brother of element 1
A D Abbreviation for the base that pairs with thymine

O You need to breathe this
V That transition metal again
I Halogen you need to prevent goitre
E It's equal to mc^2
D Schoenflies symbol for a vertical (diagonal) mirror plane between 2-fold axes
O Schoenflies symbol for an octahedral group

BCA Spring Meeting
Monday 26th – Thursday 29th March 2018

BCA 2018

THE BCA Spring Meeting is the largest UK gathering of crystallographers, of all flavours, annually. This year's Spring Meeting, BCA18, will take place at the University of Warwick from 26th until the 29th March 2018. Final preparations for the meeting are now underway. The finishing touches to the scientific programme are being agreed and this will be regularly updated on the meeting website (www.bcaspringmeetings.org.uk). The deadline for oral presentations has now passed but there is still time to submit abstracts for poster presentations – deadline for submission of poster abstracts is 17:00 GMT, Monday 26 February, 2018. We particularly encourage all early career researchers attending the meeting to consider submitting an abstract, this traditionally being an especially friendly and supportive meeting. This is an excellent opportunity for early career researchers to gain experience and exposure of your work. There is a link to the abstract submission form on the conference website.

The deadline for **early-bird registration is Friday 23rd February 2018.**

The programme for BCA18 is now available on the website including details of talks and sessions. There are a broad range of talks and topics, all prescient for crystallography today. Coupled with a readily accessible venue for all, this meeting is a great opportunity to catch up with the latest crystallographic science, and of course with your fellow crystallographers.

We are very pleased to announce an eminent list of prize and plenary lecturers as follows:

Hodgkin Lecture:
Prof. **Eleanor Dodson** (University of York)
The Joy of Seeing – in Honour of Dorothy Hodgkin

Lonsdale Lecture:
Prof. **Bill Clegg** (Newcastle University)
Distortions, deviations and alternative facts: reliability in crystallography

BSG Plenary:
Prof. **Ilme Schlichting** (MPI Heidelberg)
Protein structure and dynamics using X-ray free-electron lasers

CCG Plenary:
Prof. **Jonathan Nitschke** (University of Cambridge)
Crystallographic snapshots of soluble metallosupramolecular capsules

IG Plenary:
Prof. **Susan Reutzel-Edens** (Eli Lilly)
Predicting Polymorphism: Prospects, Progress and Perspectives

PCG Plenary:
Prof. **Nicola Spaldin** (ETH Zurich)
From Materials to Cosmology: Studying the early universe under the microscope

The traditional early-career prize session will be held on the afternoon of Wednesday 28th March. Throughout the rest of the program there will often be three sessions running in parallel in addition to a range of workshops. Brief details of the planned sessions are below, along with some practical information concerning deadlines and abstract submission. Further details and updates are available from the BCA Spring Meetings site: **http://www.bcaspringmeetings.org.uk/**.

We very much look forward to seeing you at Warwick University in Coventry.

Leo Brady
Programme Committee Chair

Biological Structures Group (BSG)

BSG Session (1): Membrane and multi protein complexes
Chair: Alex Cameron (University of Warwick) & *Kostas Beis* (Imperial)

Keynote: **Simon Newstead** (Oxford)
Understanding ligand recognition in membrane transporters

Protein assemblies, particularly those embedded within membranes, are crucial to our understanding of cellular function. They are also frequently the targets of many drugs. This session will focus on the latest advances in this very challenging area of crystallography.

BSG Session (2): Crystallisation of macromolecules
Chair: Naomi Chayen (Imperial College)

Keynote: **Terese Bergfors** (Uppsala University)
Looking for the needle in a haystack: protein crystallization screening strategies for academic laboratories

The past two decades have seen remarkable advances in the miniaturisation, automation and analysis of crystallization experiments. However, production of high quality crystals of proteins and other bio macromolecules persistently remains a major hurdle to structure determination. The focus of this session is on strategies, techniques and tools for obtaining useful crystals for x-ray crystallography.

BSG Session (3): Structural dynamics and time-resolved crystallography
Chair: Mike Hough (University of Essex)

Keynote: Dr. **Jörg Standfuss** (Paul Scherrer Institut)
Time-resolved Serial Crystallography of Bacteriorhodopsin using Synchrotrons and X-ray Lasers

Macromolecular crystallography typically provides structures that are averaged over many molecules and over the time taken to measure the diffraction data. However, proteins are dynamic, sample many functionally-relevant conformations, and undergo time-dependent structural change, e.g. through an enzymatic cycle or signalling pathway. This session will focus on the exciting science made possible by developments in structural dynamics and time-resolved X-ray crystallography using synchrotron and free-electron laser sources. Contributions describing these and other structural time-resolved methods or computational simulations are welcomed.

BSG Session (4): New instrumentation
Chairs: Pierre Aller & *Anna Warren* (Diamond Light Source)

Keynote: **Tim Grüene** (Paul Scherrer Institute)
Application of 3D Electron Diffraction to Organic and Macromolecular Crystallography

Crystallisation is often the bottleneck when it comes to obtaining a crystallographic structure, due to the difficulties in obtaining crystals of suitable size for diffraction experiments. To overcome issues of getting decent sized crystals or crystals in the first instance, new instrumentation and techniques are being developed to help the user community get the most out of their samples. New beamlines at synchrotrons are maturing to accommodate smaller and smaller crystals for either regular crystallography or serial crystallography. XFEL instruments, cryoEM and microED are becoming more popular as either an alternative to regular crystallography or to obtain complementary data. This session will focus on the scientific opportunities offered by the development of new instrumentation, and how these are aiding the crystallographic community.

BSG Session (5): Protein structure and human disease
Chair: Svetlana Antonyuk (University of Liverpool)

Keynote: **Ravi Acharya** (Bath)
Molecular functions of human Angiogenin

Changes in protein structure are associated with many human diseases. Whether studying familial disease, viral invasion or drug resistance, proteins are at the centre of nearly all therapeutic strategies. The focus of this session is on recent discoveries in targeting proteins to alter neurodegeneration in ALS, Alzheimer's and Parkinson's diseases, to understand disease mechanisms, to prevent adverse drug reactions, and recover from viral and parasitic invasion or antibiotic resistant bacteria.

BSG Session (6): Ligand binding
Chair: Atlanta Cook (University of Edinburgh)

Keynote: **Richard Bayliss** (University of Leeds)
Structures that illuminate Aurora-A kinase

The binding of ligands (peptides, nucleic acids, small molecules) to proteins is essential for the formation of protein complexes, allostery, enzyme catalysis and signalling. In turn, the ability of proteins to bind other molecules very specifically is exploited in drug discovery. Structural studies of ligand bound complexes are essential to understanding the rules of recognition and specificity, which will be the focus of this session.

Chemical Crystallography Group (CCG)

CCG Session (1): Chemistry in action (time resolved crystallography)
Chair: Claire Murray (Diamond Light Source)

Keynote: **Sam Ching** (University of Liverpool)

The inherently active nature of chemical reactions means crystallography is perfectly placed to (quit literally) shed light on how molecules move, bonds break and structures stretch or shrink. This session will explore cutting edge experiments being explored in labs and at central facilities as well as advances in in situ insight.

CCG Session (2): Molecular Machines & Rotaxanes
Chair: Stephen Moggach (University of Edinburgh)

Keynote: Dr. **Paul McGonigal** (Durham University)
Excited-State Aromatic Interactions in the Aggregation-Induced Emission of Molecular Rotors

Following the Nobel Prize awarded to Feringa, Sauvage and Stoddart in 2016, this session will highlight recent advances in the area of molecular machines. These fascinating materials and their properties will be the cornerstone of the session, highlighting the role of crystallography in the analysis and development of this research area.

CCG Session (3): Surfaces and polymorph selection
Chairs: Iain Oswald (University of Strathclyde) & *Cheryl Doherty* (Pfizer)

Keynote: **Jerry Heng** (Imperial College)
Template Induced Crystallisation for Polymorph Selection and Protein Crystallisation

Surfaces play a significant role in phase transformations and isolation of new polymorphic forms of materials. Whether it is through nucleation of pharmaceuticals on heterogeneous surfaces, or through the use of seeds to isolate new polymorphic forms, surfaces and their interaction with the molecule of interest pose key questions that are fundamental for us to manipulate the solid state. This session will explore the advances in our understanding of the role of surfaces on the isolation of particular polymorphs.

CCG Session (4): Electron diffraction
Chair: Andrew Stewart (University of Limerick)

Keynote: **Xiadong Zou** (Stockholm)
Automated Electron Diffraction Techniques for Ab Initio Structure Determination

This session will explore the application of electron diffraction techniques to solving a broad range of crystallographic problems for small molecule crystallographers. Electron diffraction is a very versatile tool, with multiple modes which can be utilised to explore the nano world. Electron diffraction tomography (EDT) mimics X-ray crystallography at the nanoscale for ab initio structure solution of unknown crystals. Nano beam diffraction (NBD) can be used to identify individually nano scale crystals, whereas convergent beam electron diffraction (CBED) enables the study of crystal defects and accurate determination of crystal symmetries. While scanning electron diffraction (SED) facilitates the study of polycrystalline

materials, via mapping of grain orientations, identification of multiple phases in a specimen, as well as stress and strain measurements within crystalline materials.

CCG Session (5): **Service crystallography forum**
Chair: William Lewis (University of Nottingham)

Keynote: **Amber Thompson** (University of Oxford)

A large proportion of published crystal structures are collected by service crystallographers. This session will offer an opportunity to share and discuss common issues and best practices encountered in a modern crystallography laboratory.

Industrial Group (IG)

IG Session: **Hydrates and solvates in pharmaceuticals**
Chairs: Helen Blade (AstraZeneca), *Spoorthy Dharmayat* (GSK)

Keynote: **Amy Robertson** (AstraZeneca)
Pharmaceutical Hydrates – What's the Problem?

Crystalline solvates or hydrates are frequently encountered within the pharmaceutical field and the development of functional medicines requires the need for a thorough understanding of their structural aspects along with the mechanisms of their formation and desolvation. The aim of this session is to link the critical factors important in building an understanding of solvated systems to mitigate the problems encountered when developing a solvate or a material that readily solvates. Such an understanding can be used to devise control strategies during handling, processing and storage to ensure that the desired functionality of the medicine can be achieved and maintained.

Physical Crystallography Group (PCG)

PCG Session (1): **Computational crystallography**
Chair: John Claridge (University of Liverpool)

Keynote: TBC

Computational techniques are important in both materials discovery and the understanding of the origin of their physical properties, particularly when combined with crystallographic studies. This session is devoted to computational structure prediction and materials "design" as well as the combination of computational techniques with experimental studies.

PCG Session (2): **Ferroics and multiferroics**
Chair: Mark Senn (University of Oxford)

Keynote: **Phillipe Ghosez** (University of Liege)
Multifunctional perovskite oxides : what can we learn from the atomic structure?

Ferroics are a technologically important class of materials that include ferromagnets, ferroelectrics, and ferroelastics. This session is devoted to experimental and theoretical studies that explore the relationship between structure and ferroic properties. Abstracts for talks exploring the coupling between different ferroic orderings in multiferroic materials are particularly encouraged.

PCG Session (3): **Perovskites**
Chair: Mike Glazer (University of Oxford)

Keynote: **Patrick Woodward** (Ohio State University)
Structural distortions in perovskites: Three case studies where size matters

The study of perovskites has been of increasing interest in the last 30-40 years, since they show such a large range of useful physical properties. The number of publications has been growing exponentially (approximately 22400 in 2016!). The latest discoveries centre around the discovery that so-called hybrid perovskites show a highly efficient photovoltaic effect, thus making them candidates as inexpensive solar cells. This session is devoted to the structures and properties of perovskites and perovskite-related materials.

PCG Session (4): **Functional materials**
Chair: Helen Playford (Warwick/ISIS)

Keynote: **Richard Walton** (University of Warwick)
Functional Oxides from Solvothermal Synthesis

Much of current research effort in materials science is targeted towards improving functional materials to meet the increasingly complex demands of modern society. However, this can only be done in a rational manner if the structural origins of desirable properties are understood. The focus of this session is on the use of state-of-the-art crystallography to determine structure/property relationships in functional materials, including catalysts, batteries, fuel cells, etc.

PCG Session (5): **Neutron and synchrotron techniques**
Chair: Anthony Phillips (QMUL)

Keynote: **John Duffy** (University of Warwick)
Spin-resolved momentum densities: What we can learn from magnetic Compton scattering

The range of experiments available at central facilities goes far beyond traditional diffraction measurements. This session will focus on techniques that take advantage of modern instruments and enhance or complement our understanding of crystallographic data. Such techniques might include magnetic X-ray scattering, anomalous scattering, small-angle scattering, total scattering, and X-ray and neutron spectroscopy.

PCG Session (6): **Hot topics**
Chair: Jan-Willem Bos (Heriot-Watt University)

Keynote: TBC

Session covering hot topics in physical crystallography not covered by the other session themes. This could for example focus on new developments in instrumentation and data analysis or studies of "hot" materials.

Young Crystallographers Group (YCG)

YCG Sessions 1-3 will showcase the work of the next generation of crystallographers from across the BSG, CCG, PCG and IG. We aim to provide new researchers (undergraduate to postdoctoral level) with the opportunity to present their work in a relaxed, friendly environment and to encourage discussion of their work.

YCG Session (1): **YCG Presentations**
Chair: Matthew Dunstan (University of Cambridge)

Plenary: **Serena Corr** (University of Glasgow)
New Series of Li-rich Double Perovskites as Active Materials for All Solid-State Batteries

YCG Session (2): **YCG Presentations: Failing badly – of all the things that can go wrong in macromolecular crystallography**
Chair: Sam Horrell (University of Hamburg)

Plenary: **Ivo Tews** (University of Southampton)

YCG Session (3): **Flash poster presentations**
Chair: Alex Cousen (University of Bath)

YCG Session (4): **When crystals go wrong**
Chair: Claire Hobday (University of Bath)

Plenaries: Prof. **Elspeth Garman** (Oxford)
The good, the bad and the ugly: macromolecular crystals in all their glory, and
Dr. **John Claridge** (Liverpool)
Interesting problems: aperiodicy, homometry and twining in materials

Crystals, the cause of and solution to all of the problems in your PhD. Whether your crystals consist of great big molecules, great small molecules or something inbetween we have all experienced problems with our crystals at some point. This session aims to unite the worlds of macromolecular and small molecule crystallography against a common enemy, misbehaving crystals, and give you some tips and tricks to help make them behave.

Parkin Lecture: Will be announced early in 2018.

Registration and Abstracts

Poster abstracts can still be submitted via the website; the deadline for poster abstract submissions is **17:00 GMT, Monday 26th February, 2018**.

The deadline for early-bird registration is **Friday 23rd February 2018**.

The final registration deadline is **Tuesday 20th April 2018**.

Programme Committee

Chair: **Leo Brady** (University of Bristol)

BCA: **Lee Brammer** (University of Sheffield), **Richard Cooper** (University of Oxford)

BSG: **Mike Hough** (University of Essex), **Mark Roe** (University of Sussex)

CCG: **Iain Oswald** (Strathclyde University), **William Lewis** (University of Nottingham)

IG: **Helen Blade** (AstraZeneca), **Spoorthy Dharmayat** (GSK)

PCG: **John Claridge** (University of Liverpool), **Jan-Willem Bos** (Heriot-Watt University)

YCG: **Sam Horrell** (DESY), **Matt Dunstan** (University of Cambridge)

Organisers: **Joanne McBratney**, **Nicola Hardaker** (Hg3 Conferences)


Piazza, Warwick University

BCA – BSG / CCG / IG Group Meetings 2017

Biological Structures Group (BSG) Meeting 2017

THE 2017 winter meeting of the Biological Structures Group (BSG) was held at the Cavendish Laboratory in Cambridge on 18th December. The organiser, Dr. **Katie Brown** (Cambridge), must be thanked for assembling a fascinating and excellent programme of speakers. The theme of the meeting was "The Joy and Pain of Structural Biology Research" with a request to speakers to emphasise some of the suffering that led to the success of their projects. The first session, chaired by Dr. **Claire Naylor** (Molecular Dimensions), began with a lecture by Prof. **Malcolm Longair** (Cambridge) on the history of the Cavendish with an emphasis on the 'decline and regeneration' of the laboratory from 1932 to 1953. However, the lecture could instead have been described as the 'ascent and ascent' of the laboratory, which is world-famous for its numerous Nobel laureates: Aston, the Braggs, Chadwick, Cockcroft and Walton, Maxwell, Rayleigh, Thompson and Rutherford, to name just a few. Indeed, Prof. Longair showed a staff photograph from 1932 featuring no fewer than 9 Nobel prize winners, taken at a time when the laboratory had an annual budget of £2000. However, under Rutherford's stern leadership and limited financial support, a number of notable Nobel laureates were to depart to pastures new. A substantial donation by Austin and new leadership under Lawrence Bragg led to the laboratory adopting a novel research group structure. Work going on in the background at this time included that of J. D. Bernal, D. Hodgkin and Max Perutz on X-ray crystallography of proteins, in parallel with the development of the electronic computer. Perutz hired a group whose names have an almost household ring to them, including Watson, Crick and Huxley as well as David Blow, one of the BCA's founder members. Their work on proteins culminated in structure determination of myoglobin and haemoglobin in the late 1950's. This was an extremely vivid and entertaining presentation and ended with Prof. Longair humorously describing how the structural biologists were frowned upon to the extent of being relegated to a portacabin in the laboratory grounds.

Next, Professor **Judith Howard** (Durham) gave a presentation beginning with early diffraction experiments at low temperature. Prof. Howard described her early career work with Dorothy Hodgkin on neutron diffraction studies of insulin and then moved on to her current research which includes neutron and X-ray studies of ethylene-platinum complexes. The neutron diffraction experiments were all conducted in collaboration with Dr. Sax Mason at the Institute Laue-Langevin in Grenoble, France. Prof. Howard emphasised that one of her key interests is in the development of instrumentation for diffraction studies at extremes of temperature and pressure with laser activation

Some of the speakers pictured here:
From left to right: ***Richard Henderson, Judith Howard, Randy Read, Malcolm Longair, Ben Bax*** *and* ***Tom Blundell.***

of transient processes in the sample. Her slides emphasised the range and complexity of the instrumentation she has constructed for these tasks. Prof. Howard moved on to describe studies of the mechanism of photo- and thermo-chromism of Schiff bases and a study of superconducting material at low temperature (2K) and high pressure.

Professor **Tom Blundell** (Cambridge) then gave a presentation with an interesting take on the theme of the meeting, namely the joy and pain of getting ones work published in the highest ranking journals. However, with Nature and Science featuring prominently in the many publications cited, this could perhaps have been better described as a story of 'joy and more joy'! Prof. Blundell described the structural biology of the protein called DNA-PK which consists of no less than 4128 amino acids and is involved in DNA double-strand-break-repair. Prof. Blundell emphasised how catastrophic a double-strand break in DNA could be for the cell and how the complex repair systems, which have evolved, play a vitally important role. Prof. Blundell described work on the protein Artemis which is involved in homologous recombination and non-homologous end-joining. A protein called Ku assembles on double-stranded break-ends and then the horseshoe-shaped PK protein prepares the DNA for ligation. Intriguingly structure determination required the development of methods for selenomethionine incorporation in tissue culture using human (Hela) cells which resulted in the labelling of no less than 116 methionine residues! Prof. Blundell described how cryo-electron microscopy has also been used to study this fascinating system and has shown the precise location of the Ku protein. A range of complementary techniques including SAXS, 3D-homology modelling and mass-spectrometry are used by his group. Prof. Blundell then described the structure of a fascinating scaffold-forming protein complex (XLF-XRCC4) which assembles into tubules and how a range of nano-technological techniques involving microscopic magnetic beads have been devised to study complex assembly processes. Prof. Blundell ended by describing fragment screening studies of the RAD51-BRCA complex which is involved in breast cancer. He emphasised how the referees of his proposals had maintained that the system was 'undruggable' but current studies have clearly proved this wrong with compounds having nano-Molar affinity being discovered.

Lunch provided an opportunity for attendees to inspect the commercial exhibition and also to visit the newly developed helium microscope which has provided stunning images of numerous biological systems. Dr. **David Ward** of the Cavendish must be thanked for setting aside time to demonstrate the equipment to numerous groups of interested attendees.

The first session in the afternoon, chaired by Professor **Elspeth Garman** (Oxford), began with a presentation by Professor **Randy Read** (Cambridge) on the road to *ab initio* phasing of structures by molecular replacement. Prof. Read described some of his early career research with Mike James in Alberta on the structure of *Streptomyces griseus* trypsin which he analysed by developing new molecular replacement methods based on brute-force 6D searching. As is often the case, the low homology with known structures (bovine trypsin 33%) was the cause of many problems. The poor quality of the resulting electron density map led him to devise ways of estimating the probability distribution for the calculated phases. Prof. Read then described the classical work of Sim (1959) and Luzzati (1952) in estimating appropriate weights for partially complete structures and those with errors. He described how the term, sigmaA, coined by Srinivasan contained both of these contributions and how it can be estimated from the correlation of the observed and calculated structure factors following normalisation. He then described how he was introduced to the now familiar concept of maximum likelihood by a paper by Alexandre Urzhumtsev. He also described the concept of the log-likelihood gain which indicates how much better your structure fits the data than a random atom model. Prof. Read concluded his talk by describing how with atomic resolution data it is possible to solve structures containing cysteine residues by single-atom molecular replacement using sulphur. He also expressed an ongoing interest in developing similar methods for the electron microscopy field due to the current resolution revolution which is providing structures at ever increasing levels of detail.

Next up, Dr. **Pamela Williams** (Astex) gave a detailed presentation on drug discovery focussing on cytochrome P450 2C9 which was solved with the important drug warfarin bound to it. This enzyme plays a major role in drug metabolism and is of great interest to the pharmaceutical sector. Dr. Williams began with a whistle-stop tour of the drug design process commencing with target selection, the identification of hits and hit-to-lead development followed by lead-to-candidate selection, preclinical studies and finally clinical trials. Dr. Williams also introduced the idea that it is helpful to analyse the structures of proteins that you do not want your drug to bind to (such as P450) so that you can then design features into it to prevent it binding to these unwanted targets. Cytochrome P450's have very flexible active sites, reflecting the wide range of molecules which they recognise for detoxification. The isoform analysed (2C9) is one of the major drug-metabolising P450's and the structure was solved by MAD using the absorption edge of the endogenous haem iron. Crystal twinning was overcome by co-crystallising the enzyme with warfarin. Dr. Williams emphasised that this analysis led to the structure determination of a range of other P450s. One of the curious features of the structure was the presence of a mystery ligand bound to the haem group. Since the most tractable crystal form of this enzyme possessed warfarin bound close to the haem, but not in contact with it, they developed a strategy of routinely growing crystals with this ligand present and then soaking-out the warfarin so that it could be replaced by other compounds of interest. This work was done in a partnership programme with a range of different pharmaceutical companies.

Next up, Dr. **Ben Bax** (York Structural Biology Laboratory) gave a fascinating presentation on the structure and function of DNA gyrase which is a type II topoisomerase. Type I topoisomerases are involved in single-stranded break repair, whereas type II enzymes are involved in repair of double stranded DNA breaks. The enzyme operates by making a temporary phosphotyrosine cross link with the DNA substrate. Dr. Bax emphasised that he had undertaken structural studies of this protein with a number of fluoroquinoline antibiotics bound and that these drugs stabilise the broken form of the DNA molecule by intercalating between the bases in the complex with the enzyme. Dr. Bax described how these studies have led to around 2 - 3 novel antibiotic compounds which are about to enter clinical trials. The structural studies he described were all dependent on engineering a form of the enzyme that was suitable for diffraction studies. Dr. Bax described some of the suffering he had endured in achieving these excellent results – namely that the gel-filtration column used to purify the protein became contaminated with different antibiotics and, as a result, an eagerly anticipated structure was found to have the wrong compound bound to it. Dr. Bax

emphasised the frustration encountered on finding that a year's work had not gone quite as hoped, but with utmost resolution and dedication they continued undeterred and finally obtained the required result. Dr. Bax emphasised a novel line of drug discovery involving the coupling of DNA gyrase inhibitor molecules to oligonucleotides by "click chemistry".

A much-needed coffee break allowed attendees to browse the commercial exhibition where the meeting sponsors (Bruker, Douglas Instruments and Molecular Dimensions) were present in force. Their extremely helpful and generous sponsorship of the meeting is very much appreciated.

The final session, chaired by Dr. **Katie Brown** (Cambridge), began with an impressive lecture by Professor **Janet Thornton** (European Bioinformatics Institute, Cambridge). Prof. Thornton focussed her lecture on a very notable paper which her group wrote in the early 90's about the very widely used protein structure validation program PROCHECK. Prof. Thornton left the audience stunned by emphasising that this particular paper now has well in excess of 20,000 citations. This is a truly outstanding achievement for those involved in writing it (R. Laskowski and M. MacArthur). Professor Thornton described how following her PhD in 1973 she became fascinated by the properties of amino acids which allow the polypeptide to fold and adopt it final elegant structure. She covered a brief history of studies on peptide geometry and how an understanding of the rules governing protein folding, such as the hydrophobicity of the core, were gradually developed. Prof. Thornton covered her detailed studies of beta-turns, beta-bulges and beta-hairpins as well as the curvature of alpha-helices, all of which depended on visualisation of these detailed structures. She mentioned how her group became aware that a number of protein structures had significant errors in the 1980's and how early PDB files suffered from inconsistencies in naming and notation. Prof. Thornton emphasised the importance of the Ramachandran plot in protein structure validation and showed some fabulous correlations between the proportion of residues in allowed regions and the resolution of each structure analysis. A number of these graphs had significant outliers and this began to ring alarm bells in the mid-90's when PROCHECK became available to the community.

The final lecture was given by Prof. **Richard Henderson** (Cambridge) who spoke on the many pains and joys involved in the first electron diffraction and electron microscopy studies of a membrane protein, namely bacteriorhodopsin, a light-driven proton pump. The work involved analysis of the protein forming the purple membrane patches which decorate cells of Halobacterium salinarum. Prof. Henderson covered the basic physics of his experimental approach and how he was able to derive amplitudes from electron diffraction and the corresponding phases from electron microscopy. By tilting the 2D crystals of this protein they were able to make the first low resolution (7 Angstroms) 3D reconstruction of this seven trans-membrane helical molecule in the mid-1970's (with Nigel Unwin). Prof. Henderson then emphasised the many conceptual barriers he had to overcome to extend the resolution beyond this in order to obtain a 3D molecular model with concurrent developments in cryo-EM and in imaging. The work culminated in a 3.5 Angstrom resolution structure of the protein which has led to hundreds of subsequent studies of this and other membrane proteins and large complexes and has also made him the latest recipient of the Nobel Prize for Chemistry.

This concluded an exceptionally interesting day which all attendees very much appreciated. The organiser, Dr. Katie Brown (Cambridge), is sincerely thanked for assembling such a fascinating programme.

Jon Cooper and **Shabir Najmudin**

(Photos by Amy Stares).

Joint Chemical and Industrial Group (CCG / IG) Meeting 2017

Design of Crystalline Products

THE Industrial and Chemical Crystallography Groups together ran a joint Autumn Meeting in 2017. This was held over 2 days at Downing College, Cambridge. With an excellent, and very busy, scientific programme plus enough time to enjoy very fine coffees and cakes at breaks as well as a college dinner in the evening, the meeting was very successful. Thanks to all the members, speakers and organisers.

Session 1: Crystal Engineering

Chairs: ***Iain Oswald*** (University of Strathclyde) and ***Luca Russo*** (GSK)

From left to right: Chair ***Iain Oswald*** *with speakers* ***Vijay Srirambhatla, Nick Blagden*** *and* ***Simon Lawrence.***

To kick off the meeting **Simon Lawrence** took us on a deep dive into the single and multi component crystallisation of sulfur containing materials. Tricky crystallisations were a common theme and Simon revealed the trends in motif

formation for hydrogen and halogen bonds in a wide family of structures. The influence of water and solvents in the templating or inhibition of some multi component systems were seen and finally he highlighted the key role of machine learning methods in the future, successful, prediction of cocrystal formation. **Nick Blagden** followed with his investigation of the dipeptide LEU-LEU and the problems caused by the impurity Trifluoroacetic acid in the salt forms due to the channels in the structure. He used co-crystallisation as a means to reduce the amount of impurity in the system. **Vijay Srirambhatla** finished the session with a presentation of the use of isomorphous templates in the crystallisation process and the relationship to computationally predicted metastable polymorphic forms. He presented the case of Carbamazepine Form V, a catemerically hydrogen-bonded systems, that was crystallised using structurally related Dihydrocarbamazepine.

Session 2: Pharmaceutical Product Design

Chairs: ***Peter Wood*** (CCDC) and ***Mathew Bryant*** (CCDC)

From left to right: Chair ***Mathew Bryant*** *with speakers* ***Ian Rosbottom, Kevin Back, Andrew Bond*** *and co-chair* ***Peter Wood.***

Kevin Back described how as part of the ADDoPT project, Pfizer is working with collaborators to use digital design to improve the process of moving from molecules to medicines. Kevin showed how CCDC's structural informatics tools are already invaluable in determining risk in polymorph selection and in cocrystal design, but that analysis of salts remains a particular challenge to the pharmaceutical industry. By leveraging the CSD Drug-Subset, developed as part of ADDoPT, Pfizer have been able to assess the chemical space that salts of pharmaceuticals occupy, and make predictions about their solid-state behaviour. By combining this type of database analysis with that of their own in-house database, the hope is that salts of pharmaceuticals may be able to be designed with specific properties or stabilities required.

Ian Rosbottom described how in the current pharmaceutical industry, problems with manufacturing pharmaceuticals can often arise from problematic crystal morphologies and particle properties. Through the use of the program HABIT (which uses forcefield calculations to make predictions about directionality and strength of intermolecular interactions), a study has been performed on the crystal structure alpha-PABA. Ian shows how the predicted interaction of different faces with various solvents allowed them to design a set of crystallisation conditions to control the growth rates of fast-growing faces. This has allowed for the growth of a more favourable crystal habit.

Andrew Bond began by explaining that when studying crystals, the intermediate scale between atomic level, and bulk properties is often the least well understood. Through the use of nanoindentation techniques, Andrew shows that anisotropy in the mechanical properties of crystal structures can be linked to structural features. Andrew demonstrates that crystals often arrange into domains, and that the periodicity of these domains can be detected through nanoindentation experiments.

Session 3: Early Career Session

Chairs: ***Cheryl Doherty*** (Pfizer) and ***Claire Hobday*** (University of Bath)

From left to right: Discussions led by ***Peter Wood, Claire Hobday, Mathew Bryant*** *and* ***Cheryl Doherty.***

This interactive session was quite different from our normal slots. The speakers had been asked to describe their career path and any tips or challenges to kick off a discussion, mostly focussed around identifying difficulties and some ways the BCA can help early career researchers. Firstly **Mathilde Reinle-Schmitt** described her career path from university through to a full time industrial position at Excelsus Structural Solutions, a small start-up based at the Swiss Light Source. She highlighted the importance of mentors and networks to make contacts and described how she identified the best route to a fulfilling role. This was followed by **Hamish Yeung**, currently a Fellow at the University of Oxford. Hamish described his academic career path and demonstrated the value in collaborations and where to find them. Tea break conversations and skiing holidays were shown to be an especially good source of collaborators.

This was followed by a discussion session and the audience split into two. Some broad themes that were addressed in the discussion included difficulties for early career researchers, and women in STEM particularly, such as the prevalence of short term positions, lack of flexibility in hours and location and the lack of a full time researcher (with no teaching) positions. In addition, we discussed how young researchers could make their mark by having an increased presence both with social media and making the most of conferences to discuss with more distinguished scientists and forge collaborations. The BCA can ensure we offer opportunities to all members and look for ways to be flexible to allow everyone the chance to attend/speak/contribute. We discussed how there are bursaries available for PhD students to attend the BCA spring meeting, and extending funding to PDRAs could encourage more contributions from early career researchers. The value of poster sessions and networking time at conferences (such as the autumn meeting) was highlighted as well as the open and friendly atmosphere needed to help new scientists develop their skills in this area. It was thought that making more time

for early career researchers in the main BCA meetings could help. With regards to contact with industry, the cost of, for instance active pharmaceuticals, was highlighted as being a barrier to research on relevant compounds. Industrial partners could be asked to consider ways to make this available if possible.

Overall we had a robust and very open and honest discussion. The audience participated very enthusiastically and many had a chance to speak. While several significant issues were too broad to fully address within the BCA, the chairs agree there are efforts we can make in the Industrial and Chemical groups to help on a number of fronts and we will be bringing these to the attention of our committees for consideration in future.

Session 4: Crystallisation & Crystallisability

Chairs: ***Richard Cooper*** (University of Oxford) and ***Cheryl Doherty*** (Pfizer)

From left to right: Speaker ***Mike Zaworotko*** *with Chair* ***Richard Cooper****.*

To start the second day, we were delighted to hear from **Mike Zaworotko** on crystal engineering of task-specific materials. He gave a comprehensive overview of his research in development of both conventional and ionic co-crystals for pharmaceutical formulation, followed by results of a study of targeting hydrate formation in a series of related compounds. Finally he presented a robust chiral metal organic framework which acts both as a 'crystalline sponge' for determination of structures of small molecule guests and as a stationary phase for separation of enantiomers.

The next session focused on crystallisation and crystallizability and the first speaker was **Aurora Cruz-Cabeza**. She explained how kinetic nucleation and growth parameters can reliably be extracted from multiple recrystallization experiments and in data from a series of compounds showed that aromatic stacking interactions had the most influence on nucleation and growth rates.

Andrew Tatton next introduced the use of NMR to correctly identify crystal structures for samples were single crystal diffraction has not been successful. He showed examples where the use of CASTEP and solid state NMR data can be combined to pick out the right powder or predicted crystal structure solution for complex materials.

To round off the session **Melissa Birch**, from Pfizer, provided a glimpse into large scale chemical crystallisation processes. She showed the production of a wide range of particle shapes, sizes and physical properties from the same crystal form by expert manipulation of the crystallisation parameters on scale. She also demonstrated the importance of understanding supersaturation within your system to provide the control necessary to develop a robust and reproducible process.

Session 5: Non-Ambient Diffraction

Chair: ***Clare Hobday*** (Bath)

From left to right: ***Charlie McMonagle*** *with* ***Claire Hobday*** *and* ***Malcolm Halcrow****.*

After lunch on Day two, Session Five commenced with two speakers Prof. **Malcolm Halcrow** (University of Leeds) and **Charlie McMonagle** (University of Newcastle). Prof. Halcrow gave a talk entitled "Insights into the t1/2 vs t(liesst) Relationship from an Isostructural Series of Spin Crossover Solvates" where he demonstrated the diverse spin-crossover behaviour of Fe(II)complexes. These complexes are becoming increasingly popular for device and sensor applications, and in soft materials, that make use of their switchable colour, paramagnetism and conductivity. In their high-spin state, the complexes are pale and transparent whereas in low-spin their colours are dark and opaque. He showed an interesting complex which undergoes an incomplete (50 %) spin transition upon cooling which results in a crystallographic phase transition from $P2_1/c$ (Z' = 4) to $P2_1$ (Z'= 24). The low temperature phase contains a mixture of high-spin and low-spin molecules, which are grouped into triads. He also highlighted the effect of crystal packing and density on cooperative switching mechanisms.

Charlie McMonagle ended the session with his talk entitled "A Sapphire Capillary Pressure Cell for the Small Molecule Beamline I19 at Diamond Light Source". He introduced a new pressure cell for diffraction experiments in a pressure range which is not commonly studied. I19 has a great gas-cell set-up to probe single crystals with gases up to 200 bar – interesting for studying adsorption properties in porous materials or phase transition in soft materials. In addition, I19 has an easy set up for diamond-anvil cell experiments (between 1 kbar and 100 kbar) useful for probing phase transition in pressure sensitive materials. Charlie introduced a cell which bridges the gap between these two pressure regions, allowing measurements from 1 bar to the kbar region. The design is easy to use and he showed us case studies on small molecules and porous materials. The case studies highlighted the versatility in the materials which could be studied, as well as the pressure transmitting media which could be applied – n-pentane, isopentane, water and methanol. The use of a single crystal sapphire capillary makes the diffraction data cleaner than quartz capillaries and allows for more regions of reciprocal space to be sampled than in the diamond-anvil cell. The cell is now available for users on I19 at Diamond Light Source.

Session 6: Property Control & Prediction

Chairs: ***Andy Moloney*** (CCDC) and ***Luca Russo*** (GSK)

From left to right: Chair ***Andy Moloney*** *with* ***Jack Evans, Graeme Day, Monika Warzecha*** *and co-chair* ***Luca Russo****.*

The final session, closing the meeting, was entitled 'Property Control & Prediction', featuring three inspiring talks that were well aligned with the theme. The first was by **Monika Warzecha** from Strathclyde University on the 'Direct Observation of Templated Two-Step Nucleation Mechanism during Olanzapine Hydrate Formation'. This demonstrated the potential of AFM to harness mechanistic information on nucleation and, more generally, the capabilities of AFM to monitor solid-state form processes.

The second talk was by **Jack Evans** from Chimie ParisTech, on 'Predicting the Properties of Porous Crystals using Multi-Scale Simulation' and focussed on the modelling of the DUT-49 MOF and its unusual negative gas absorption behaviour, by means of DFT calculations and Molecular Dynamics.

The session was closed by **Graeme Day** from Southampton University with a fascinating talk proposing a paradigm shift entitled, 'From Crystal Structure Prediction to Energy-Structure-Function Maps: Computational Guidance for Functional Materials Discovery'. Graeme's work, recently featuring in *Nature*, proves that whilst challenges in Crystal Structure Prediction are still ongoing, the available tools seem mature enough to support the design of crystalline products with targeted properties, such as very low density MOFs.

Cheryl Doherty
Pfizer R&D

Yue Deng, winner of the fifth PANalytical Award

The annual award recognizes innovative X-ray analytical research by young scientists.

18 SEPTEMBER 2017, Almelo, the Netherlands. The PANalytical Award 2016 has been won by Dr. Yue Deng, a former PhD student at the University of Bath (UK) and the University of Picardie (Amiens, France). His article about fast lithium-ion conduction in solid electrolytes was highly rated by the selection committee who especially mentioned the excellent quality of the comprehensive work described in the paper. The winning article was selected from a record number of more than 100 contributions from scientists all over the world.

Dr. ***Yue Deng*** *(centre), with his PhD supervisors Prof.* ***Christian Masquelier*** *(University of Picardie, left) and Prof.* ***M. Saiful Islam*** *(University of Bath, right).*

Yue Deng and his co-authors were delighted by the good news. He said: *"This award is a great acknowledgement for the value of our work, and a great encouragement for me to apply my knowledge of diffraction and crystallography in my career".* He will receive the PANalytical Award in Shanghai (China) where he is currently working. More details about the award-winning article and its author can be found on the Malvern Panalytical website.

The prize was decided by a selection committee that included Malvern Panalytical scientists and approved by established researchers unaffiliated to Malvern Panalytical. Their decision was made especially difficult by the high quality of the submitted articles. The jurors have nominated two close runner-up's: **Nathan Bossa** *et al.* for their article about the characterization of the pore network of a leached cement paste by computed tomography and **Clément Falaise** and **May Nyman** for their work about the aqueous self-assembly of uranyl peroxide nanocages.

German Crystallographic Society Annual Meeting 2017

IN recent years this meeting has taken place mid-March. The 2017 meeting at the Karlsruhe Institute of Technology was scheduled after the start of springtime, 27-30 March, and the weather in this corner of southwest Germany provided a tempting series of warm sunny afternoons. It required a combination of German diligence and interesting presentations to keep participants indoors attending sessions.

Ilme Schlichting

The first plenary lecture started things off with exciting developments involving XFEL. Under the title "Protein structure and dynamics using X-ray free electron lasers" **Ilme Schlichting** (Max-Planck-Institute for Medical Research, Heidelberg) presented some recent triumphs but did not gloss over the difficulties. XFELs offer much greater brightness than is achievable with a synchrotron. They are particularly suitable for time-resolved studies and outrunning radiation damage. They are characterised by low stability, high adjustability and single-user operation. Synchrotrons have exactly the opposite characteristics. XFELs have lots of controls, which are not orthogonal. Therefore "every run is an experiment, never merely a measurement". The XFEL beam has the SASE spectrum superimposed, which changes all the time. The small randomly orientated crystals may receive the full beam or just be grazed by it. Crystals to be injected into the beam may float or sink; rotating the injector assures a homogeneous suspension. A successful study examined binding of a ligand (carbon monoxide) to very small crystals of myoglobin (Mb). Photodissociation of the MbCO complex can be achieved with quantum yield nearly 1 and is fully reversible in about 2 ms. The delay between optical pump and X-ray probe pulses can be varied. Within 0.2 ps the CO dissociates fully and the heme group becomes domed with Fe 0.2 Å out of plane. Subsequently the photolysis spreads out like an earthquake, and large structural changes are observed after 100 ps. Diffraction before destruction works!

Microsymposium 02 introduced us to some weird and wonderful compounds as it covered structural chemistry under non-ambient conditions. **Maxim Bykov** (Bayreuth) talked about "Novel nitrogen-rich iron nitrides synthesized at high-pressure high-temperature conditions". Metal-rich nitrides can make permanent magnets, e.g. γ-$Fe_{10}N_2$. Experiments on FeN at 293 K and 1900 K show similar structure at the two temperatures, only affected by thermal expansion. Marcasite-type FeN_2 is easily compressible along the *c* axis but rigid along *a* and *b*. FeN_4 at 135 GPa and 2700 K has polymeric nitrogen chains. **Lkhamsuren Bayajargal** (Frankfurt am Main) told us about "Synthesis of binary hafnium oxides at high pressures and high temperatures". Studies in a diamond-anvil cell at Petra III demonstrated the formation of Hf_6O and Hf_8O_7 from Hf and HfO_2. **Benedikt Petermueller** (Innsbruck) described "High-pressure synthesis and crystal structure of a new orthorhombic modification of Ir_4B_5." With starting materials of Ir and B in proportions 1:3 high-pressure high-temperature synthesis formed the title compound, unexpectedly featuring layers of boron atoms coordinated with Ir to form columns. This structure is stable up to at least 25 GPa. **Gregor Hofer** (Zurich) presented "The photo-induced and temperature reversible single-crystal-to-single-crystal transformation of a two-dimensional polymer". A trifunctional monomer can be partially polymerized, leading to sheet stacks and monolayers. Polymerization could involve neighbour encouragement, be random or exhibit neighbour inhibition. The latter seems to apply to the system studied, whether undergoing polymerization or depolymerization. Used as a solvent, 2-cyanopyridine becomes incorporated into the polymer. **Dennis Wiedemann** (Berlin) examined "Diffusion pathways in ion conductors – making the most of neutron diffraction data". Lithium ion diffusion is important in battery design. Studying it by neutron diffraction has pitfalls: synthesis, which may lead to bi-phases; sample degradation; mismeasurements; modelling errors; evaluation flaws. In this series of compounds neutron diffraction gives framework crystal structures, facilitating topological analysis by Voronoi-Dirichlet partitioning. Maps of scattering-length density can be produced, analogous to electron density with X-ray data. Pathways for rapidly migrating Li ions in $Li_2Ti_3O_7$ were identified. **Stefan Schwarzmüller** (Leipzig) concluded the microsymposium with "Thermoelectric properties and atom mobility in argyrodite-type $Cu_8GeSe_4Te_2$". High electron mobility can occur through the rigid substructure, but there also are mobile atoms. The $MgCu_2$ structure type has a substructure of Mg and vertex-sharing Cu. Introduced Se atoms join the rigid substructure forming tetrahedra, and the mobile substructure has Cu sites with occupancy factor 0.24 . Substitution of Se by Te increases electron conductivity by some orders of magnitude.

The prestigious Laue Talk was given by **Francesca Fabbiani** (Göttingen) on the subject of "Investigating and understanding drug polymorphism: how high-pressure crystallography can help". Francesca began by laying out the wide variety of fields where high pressure is relevant: planetary science, synthesis of novel materials, biological effects of pressure, and industrial

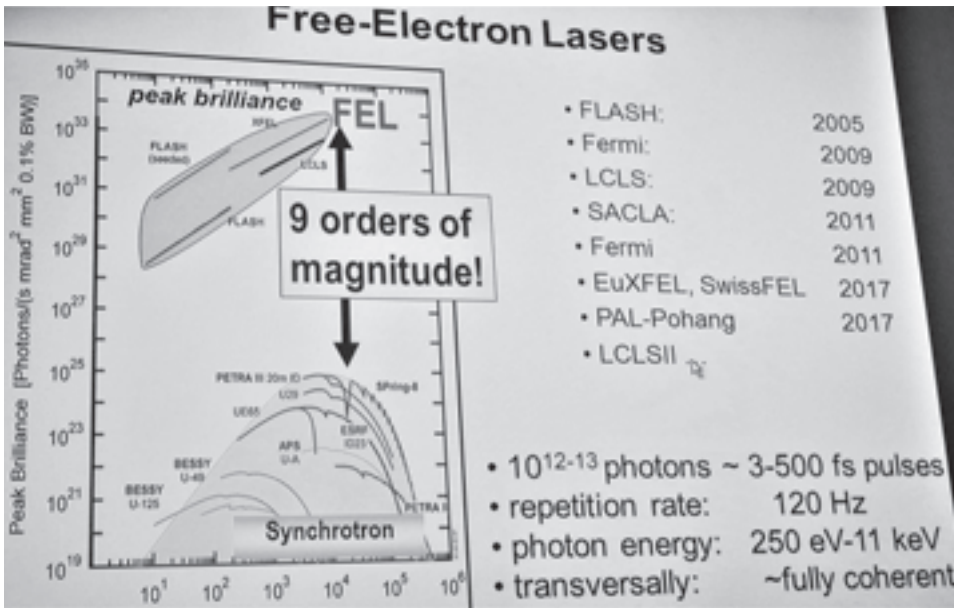


Illustration by ***Ilme Schlichting*** *comparing XFELs with synchrotrons, together with worldwide examples of XFELs.*

applications. In the pharmaceutical industry different polymorphs, which may appear at various stages of a drug's life, affect features which have implications for regulatory requirements and intellectual property. Extending the screening landscape to explore p-T space ensures that *in situ* conditions of manufacturing processes are recreated. Within a Merrill-Bassett diamond-anvil cell single crystals or powders can be loaded, or crystals can be grown from the melt (beware of decomposition) or solution. An example from Francesca's group is the very water-soluble GABA, known to have 2 polymorphs at ambient conditions, where there is no driving force for hydrate formation. However, GABA.H_2O was grown from aqueous solution at 0.5 GPa. Beta-cyclodextrin inclusion complexes start with Form I of the 1:1 complex. Crystallization at 0.8 GPa produced Form V, a 1:0.333 complex with 24 water molecules per complex. An example of rational polymorph screening is provided by dalcetrapib, which has polymorphs A and B under ambient conditions. The crystal energy landscape shows that A is most stable, B most dense; but there are others with a better combination of stability and density. Crystallization from THF at 0.45 GPa gives Form C, which is close to the prediction from theory.

Another plenary lecture presenting dramatic technical advances was "MicroED opens a new era for biological structure determination" by **Tamir Gonen** (Ashburn, VA, USA). Macromolecular electron crystallography was first demonstrated on catalase in 1937. A long series of innovations has eventually led to *ab initio* structure determination of biological macromolecules. Electrons have advantages over X-rays. With X-rays, for every 1 photon usefully scattered there are 10 inelastically scattered, leading to radiation damage. With electrons, the ratio is 1:3 . Furthermore, the much stronger interaction of electrons with matter means that smaller and thinner crystals can be used. There is a big problem with electron diffraction (ED) from 3D crystals. For X-rays of wavelength typically on the order of 1 Å the scattering angle is much larger than for electrons, typically 0.025 Å. In the latter case the Ewald sphere is almost flat, making indexing very difficult. MicroED allows much lower doses, so that multiple diffraction patterns can be recorded from the same crystal. The technique was developed on lysozyme crystals typically 0.4 mm across, but 150 nm thickness was sufficient. The critical dose leading to crystal death is *ca*. 9 e / $Å^{3,}$ and just 3 crystals may be enough to cover the full reciprocal space. Continuous rotation, recording data as a movie, solves the problem of partially recorded reflections. Since 2013, 37 protein structures have been determined by microED, 12 by direct methods at resolution 1.1 Å. An impressive example is the toxic core of α-synuclein, implicated in Parkinson's disease, determined from crystals 50 nm thick and wide that were invisible because they were smaller than the wavelength of visible light!

The 2018 meeting will take place earlier in March (5th-8th) in the more northerly location of Essen. Therefore, I wouldn't be completely surprised if participants got some snow crystals to broaden the discussion further.

Carl Schwalbe

1st Pan-African Conference of Crystallography

THE First Pan African Conference of Crystallography (PCCR1) was held at University of Dschang in Cameroon from 06 to 10 October 2016. It was an enjoyable scientific meeting which welcomed thousands participants around the world, especially from Africa.

Thanks to the financial support from the event's partners, especially British Crystallographic Association, I was able, with my student **Marielle Yasmine Agbahoungbata**, to attend this conference on behalf of the University of Abomey-Calavi (Republic of Benin). Many activities such as oral communications, posters exhibition, round tables and travel tour have been done. This report aims to give a summary of the event and some appreciations.

Overview on the activities

Opening Ceremony:

The opening ceremony of PCCR1 was held on 6th October, 2016 after participant registration and the visit of the famous "Musée des Civilisations". The opening lecture was on the theme "From molecule to crystal".

Oral communications:

The global theme of the conference was "Crystallography for sustainable Development in Africa". There was seven technical sessions around this thematic. Basically, participants did an oral presentation on their research work in the suitable session. With my student, we did, each of us, an oral communication in session 5:

Inorganic materials and mining industry. My presentation was on "Characterization of Benin's clays used in ruminates feeding: complete determination of the smectites contained in these clays." while the one from Marielle was on "Development of novel visible light active photocatalyst N-doped TiO_2/Clay for wastewater purification."

Our communication has focussed especially on the use of X-Ray Diffraction technique for mineral clays and clay based materials characterization. Indeed, clays are abundantly available in Benin but not well valorised due to the lack of scientific studies on them. Throughout our work, different kind of mineral clays have been identified from raw samples by using XRD. These minerals were successfully used as supports in photocatalysts development and as adsorbent for remediation of methane emission according to their crystallographic properties.

Other oral presentations were given in many research fields such as crystal engineering and structural chemistry, inorganic materials and industry minerals, crystallography for life science, crystallography data bases and facilities for emerging countries.

Poster communications:

As far as this activity is concerned, many posters have been exhibited during the conference. Various topics (from crystals growing technology to their applications) were developed. Usually, the visit of posters was organised during the breaks and the evening at the end of oral communication sessions and allowed all participants to meet each other and discuss around posters. This was also completed by the exhibition of the most recent developments in commercial instrumentations.

Round tables:

Two important round tables were organised and devoted respectively to "Crystallography as vehicle to promote science in Africa and beyond" and "Equipment for African laboratories and the African light source, AfLS." It was an opportunity to share with others African crystallographers about the state of education and research infrastructure in Africa.

Travel tour:

On the last day of the conference we went to Limbé for an enjoyable local tour. In a friendly atmosphere we visited the beach and some mountains.

Academic and social Impacts:

The first Pan African Conference of crystallography has been an excellent opportunity to meet and exchange with many researchers and crystallographers from different Universities.

The oral communications as well as posters exhibitions allowed us to deepen our knowledge in many fields especially in crystal engineering. We acquired some skills regarding the use of X-Ray Diffraction in single crystal characterisation and the crystal structure resolution. Our oral presentation allowed us to share with participants. These exchanges were very fruitful and will be useful for improving our research work.

We have discovered and enjoyed Cameroon culture throughout the Limbé travel tour and the visit of "Musée des civilisations".

Conclusion:

Participation to PCCR1 has been a great satisfaction for us regarding the fact that we acquired many benefits (academic, social and cultural). The various lectures received allowed us to discover more applications of crystallography. Thus, in the short term, I will put the acquired knowledge for the benefit of my student's research to let them better complete their work. Also, this experience will be a trump for our contribution to the future organization of Pan African Conference of Crystallography in our home University.

Acknowledgements:

We express our deep gratitude and thanks to all partner especially the British Crystallographic Association for its financial support which permitted our participation to the first Pan African Conference of Crystallography.

We warmly thank the PCCR1organisation committee for its very good and successful organisation.

Our special thanks to Dr **Patrice Kenfack**, Prof. **Ignace Tonle Kenfack** and Prof. **Claude Lecomte** for their solicitude.

Prof. **Etienne Sagbo**

I ATTENDED the First Pan African Conference of Crystallography in Dschang (Cameroon) on 6-10 October, 2016. I was funded by the British Crystallographic Association (BCA) for the Senegal- Cameroon-Senegal trip and stay as well.

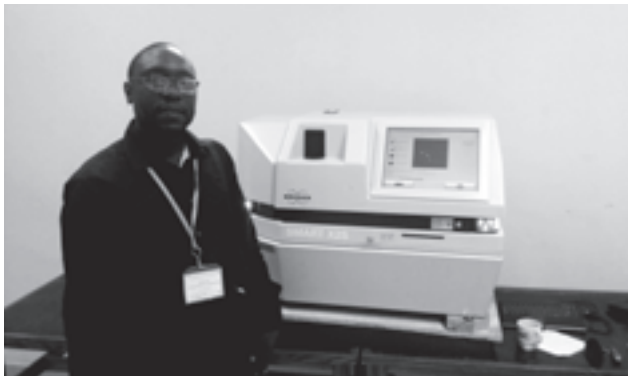
During the stay, I was invited to present my research papers. My poster is one of the best, nominated by the Scientific Committee and a prize has been designated to me in this sense. This conference allowed me to meet researchers from many countries. I would like to thank the British Crystallographic Association (BCA) for its funding. I would like to thank the university of Dschang (Cameroon) for the warm welcome.

Insa Badiane
PHD Student (Senegal)

Insa receiving his award.

Award winners.

Poster presentation sessions.



Picture taken next to the DRX single-crystal diffractometer.

Important Announcements

Nominations for the 2018 Bertaut Prize

THE European Crystallographic Association (ECA) and the European Neutron Scattering Association (ENSA) invite nominations for the Erwin Felix Levy Bertaut Prize 2018. The Prize is awarded in memory of the scientific achievements of the late Erwin Felix Lewy Bertaut, which are cornerstones in both crystallography and neutron scattering. The Bertaut Prize is awarded to a young scientist (up to 8 years after finishing her or his PhD thesis) having a clear affiliation with the ECA/ENSA region, in recognition of notable experimental, methodological or theoretical contributions to the investigation of matter using crystallographic or neutron scattering methods.

Nominations for the Bertaut Prize may be submitted by European scientists as individuals (self-nomination excluded) or on behalf of a group.

Nominators may be:

(i) an ECA/ENSA Individual Member or

(ii) any person from a National Member of ECA/ENSA or

(iii) any Corporate Associate Member (CAM).

The nominator must ensure a signed acceptance of the nomination by the nominee. Nominations should include the motivation for the award, a brief curriculum vitae of the nominee and a short list of major publications. Letters of support from authorities in the field are accepted.

Nominations for the prize will be treated in confidence and, although they will be acknowledged, there will be no further communication. The candidate will receive the Bertaut Prize at the European Crystallographic Meeting 2018 in Oviedo (ECM31) and present a lecture on this occasion. Nominations are now open and will close on **April 20th, 2018**.

Nominations must be sent to the ECA Vice President at the address: **vice.president@ecanews.org**

Editor's note: this notice is featured in *Crystallography News* this year because I think that a British candidate may stand a better chance while scientific links with Europe remain intact.

New Ionising Radiation Regulation

ONE of our Corporate Members, Scimed, has sent out the following communication for the benefit of the UK crystallographic community.

This is an important communication if you are an XRF (X-ray Fluorescence) or XRD (X-Ray Diffraction) user.

You may have heard that the Ionising Radiation Regulation 1991 (IRR 91) has been reviewed and will be superseded by IRR2017. This regulation governs users of any kind of radiation source, including X-ray tubes.

All benchtop and floor standing XRF's and XRD's with the X-rays enclosed in a sealed chamber fall in the lowest category of the regulation, while hand held XRF's will follow a stricter set of rules. The XRF's and XRD's that SciMed has supplied during the past 30 years such as the Asoma, Spectro, Rigaku and Hitachi (SIINT) spectrometers fit in the same category.

Unfortunately, despite the fact that the new rules were intended to come into force from January 1st 2018, at the time of writing in December 2017 they were still at the draft stage! However, the regulations are now in effect.

As a concerned provider, we wanted to make you aware of the current state of the draft, which will provide some guide lines of the changes that might affect your compliance.

The most notable change is the way the HSE is informed about the uses of ionising radiations moving from a single notification system to a three-tier system consisting of notification (for low risk users), registration (for medium risk uses) and consent (for specified practices); the use of the X-ray analytical equipment falls into the registration tier. It is compulsory for all users of ionising radiation to inform HSE using the new three tier process irrespective of any previous notifications made in the past. HSE have created a web-based portal for the three-tier system and we understand this should be available from the 4th of January 2018; the company will then have until the 5th of February 2018 by which to register the use of the X-ray analytical equipment. HSE are making a nominal charge of £25.00 for registration – this will be charged at the time of making the online application.

Summary of other anticipated changes:

- The recording and analysis of significant events, and any events which trigger the use of contingency plans, will be required. Most companies will already do this as part of their own safe system of work (identifying corrective & preventative actions etc.). Notification of such an event will not be required by the HSE under IRR17, but RIDDOR reporting requirements will remain unchanged.

- The retention period for dose records will be reduced from 50 years to 30 years.
- The eye dose limit will be reduced from 150 mSv to 20 mSv per annum. This should have no impact on companies which undertake 'whole body' dosimetry.
- The notification and intervention level for radon will change from the present 400 Bq/m^3 averaged over 24 hours, to 300 Bq/m^3 averaged over one year. The HSE are of the opinion this change will have no impact.
- An estimate of doses to the public will need to be completed by all employers who carry out a radiation practice. This should mainly impact on companies who transport radioactive material and / or those undertaking site radiography.
- The term 'Radiation Employer' will cease to exist under IRR17, and be replaced with 'an employer who carries out a practice that involves ionising radiation'.
- There may be a move away from the current 'RPA 2000' approval scheme. This will be discussed by professional bodies and could ultimately result in a combined scheme for RPA, MPE (Medical Physics Experts) & RWA (Radioactive Waste Advisors). James Taylor (HSE) indicated that a change could be implemented for RPA approval.

Please contact your Radiation Protection Advisor who should be able to formally guide you through these changes.

Whilst we are not authorised as a manufacturer's representative to directly advise users, do feel free to get in touch with any questions you might have, and we will point you in the right direction.

Paul Vanden Branden
[Paul@scimed.co.uk]
SciMed XRF

XRF-XRD After Sales Co-Ordinator:
bev.whyman@scimed.co.uk

Radiation Safety Officer / XRF Senior Service Engineer:
rob@scimed.co.uk

CryoEM section launched in IUCrJ

IUCrJ, launched by the International Union of Crystallography (IUCr) in 2014 as an open-access journal publishing high-quality articles across the structural sciences, has included cryoEM since 2015 as part of its biology and medicine section. Recognising the structural biology revolution brought about by cryoEM, the IUCr is pleased to announce a fully dedicated section on cryoEM in IUCrJ. Sriram Subramaniam (NIH, Bethesda, MD, USA) is at the helm as the Main Editor and he, together with Werner Kühlbrandt (MPI, Frankfurt, Germany) and four new Co-editors – Esther Bullitt (Boston University, MA, USA), Lori Passmore (MRC-LMB, Cambridge, UK), Stefan Raunser (MPI, Dortmund, Germany) and Fei Sun (Institute of Biophysics, Beijing, China) – will attract high-quality papers and champion IUCrJ as the natural home for cryoEM results and breakthroughs in instrumentation and methods developments. *"Our aim"*, said Dr Subramaniam, *"is to have a long-term impact in structural biology by providing a forum for rapid publication of important results in the cryoEM field."*

IUCrJ is the most comprehensive science journal of the IUCr and has already received an impact factor of 5.8. It benefits from fast publication, robust peer review, expert technical editing and, being open access, unlimited readership. **Samar Hasnain** (Max Perutz Professor of Molecular Biophysics at University of Liverpool, UK), Editor-in-Chief of IUCr Journals, is pleased to launch this dedicated section on cryoEM, which he regards as *"the method of the decade for structural biology."* **Richard Henderson** (MRC-LMB, Cambridge, UK), who has been a member of the journal's Editorial Advisory Board since 2015 and who recently shared the 2017 Nobel Prize in Chemistry with **Jacques Dubochet** and **Joachim Frank** for the development of cryoEM, applauded the move: *"As cryoEM increases in power we welcome the broadening of the scope of IUCrJ so that the different methods become more fully integrated."*

B. T. M. (Terry) Willis
(1927 – 2018)

TERRY Willis left us on 18th January 2018 after a long and active life. Terry obtained an honours degree from Cambridge in 1948, and a Ph.D from Royal Holloway, University of London in 1951 with Bernal and Tolansky as his supervisors. After working with X-rays for 3 years at the GE Research Laboratories, he was recruited by George Bacon to come to Harwell. Within 2 years the new reactors DIDO and PLUTO were operating, and Terry set about building a 4-circle diffractometer to measure single crystals. With the help of Ulrich Arndt, he persuaded Ferranti to construct such a machine and it was operating with punched paper tape by 1960. In 1966, Terry and Arndt published a book "Single Crystal Diffractometry", which was reprinted in paperback in 2009.

Exploiting the ability of neutrons to detect light atoms in the presence of heavy ones, Terry fastened on to the idea of using neutrons to examine uranium dioxide, which had by then become the nuclear fuel of choice. This led to a number of pioneering experiments, including the first publication (in *Nature* 1963) of the structural changes when UO_2 takes up additional oxygen. Terry continued his love affair with the many forms of uranium oxides for the rest of his life, working more recently with the high-resolution powder diffractometers at ISIS. He proposed the so-called "Willis clusters", and these are still the subject of research today.

Terry and **Peter Egelstaff** (1925 – 2015) became the primary exponents of opening the Harwell neutron scattering facilities to university researchers. He introduced many to Harwell who went on to become leaders in the field including **Dorothy Hodgkin** (1910 – 1994) and **Maurice Wilkins**. Terry encouraged many of Hodgkin's students and co-workers to come to Harwell and use neutrons. **Judith Howard** recalls of her time working with Terry: *"He was hugely supportive and patient with an unbelievably 'green' neutron student from a chemistry department. He almost converted me to a physicist during that time and I learnt to build equipment as well as to interpret neutron data".*

Terry's ongoing research from the 1960s led to another book "Thermal vibrations in crystallography" with **Arthur Pryor**. **Hugo Rietveld** was a frequent summer visitor to see Terry at Harwell where they discussed the profile fitting method. **Alberto Albinati** came from Milan, and **Noriaki Kato** from Japan. Terry himself was a visitor to Denmark, India, Switzerland, Pakistan and Japan.

In 1965 **Mick Lomer** (1926 – 2013) head of the Materials Physics Division at Harwell asked Terry to organize a Summer School to help train its many external users. The world's first "Summer School on Neutron Scattering" took place at Harwell in 1966 with **Gordon Squires** giving the theory lectures, which he later turned into one of the best texts on the introduction to neutron scattering. 50 years later these schools, now moved to Oxford, still take place every 2nd year. In re-starting the schools at Oxford in 1979, Terry joined forces with **Colin Carlile** – and they produced yet another important book: Willis and Carlile, (2009), Oxford University Press, (2009). From the many school photographs we estimate that the summer schools have instructed almost 1,000 students.

Terry's first wife, **Nanette**, died early, but with his second wife **Margaret**, Terry was always in attendance at the summer schools and together they entertained the students with"Tea and Croquet" on the Saturday afternoon at their home on the river in Oxford. They were certainly memorable events for all concerned, and many students were introduced to the unfathomable complexity of croquet and punting for the first time!

*(Left to right): **Alberto Albinati** (Milan), **Margaret Willis** and **Terry**.*

In 1982, Terry Willis became one of the founding members of the British Crystallographic Association, and was awarded Honorary Membership in 1999 in recognition of significant contributions to crystallographic science and the work of the BCA.

Terry left Harwell in 1984 and became a Professor in Chemical Crystallography in the Chemistry Department at Oxford University, where he continued neutron experiments right up to and beyond his retirement in 1990. His enthusiasm and generosity in collaboration was a boon to students and researchers in the laboratory, who benefited from discussing their work with him and even becoming involved in experiments and analyses with Terry and his collaborators across the world.

Terry remained great friends with students and colleagues and he and his family would often share long walks and delicious Sunday dinners with weekend visitors while they were visiting Oxford.

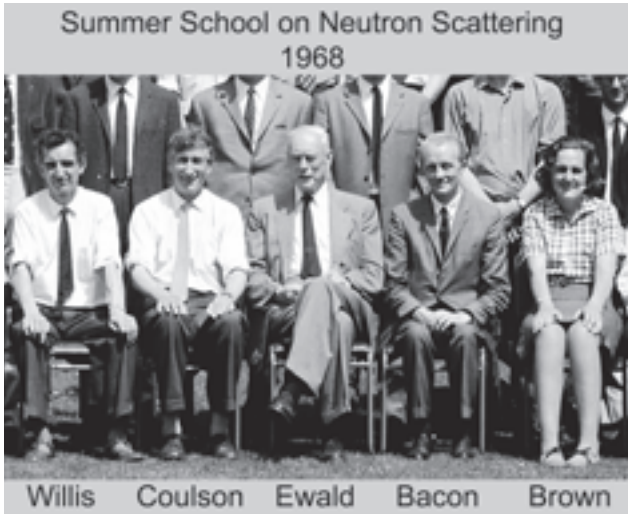
He had friends from across the globe in neutron scattering, many of whom gathered to celebrate his 70th and 80th birthdays and they too will miss a great friend and a bright mind. Terry was a brilliant physicist, a huge contributor to the neutron community and a gentle and kind man.

Terry's enthusiasm never left him; all neutrons were good neutrons. He was a good friend and mentor in his personal life and a rigorous and talented scientist in all his professional dealings. We shall greatly miss him.

Contributions from **Gerry Lander**, **Colin Carlile**, **Judith Howard** and **Richard Cooper**.

See also "Willis – a tribute" under the Harwell header on: http://neutronsources.org/about/history/literature.html and http://www.oxfordneutronschool.org/history.htm

There is a justgiving page: https://www.justgiving.com/fundraising/bertram-willis which Jon Willis has set up to raise money for RNIB which offered tremendous support to Terry over the last few years.



Meetings of interest

FURTHER information may be obtained from the websites given. If you have news of any meetings to add to the list, please send them to the Editor, c.h.schwalbe@hotmail.com . Assistance from the IUCr website and the *Journal of Applied Crystallography* is gratefully acknowledged.

5-8 March 2018
26th Annual Meeting of the German Crystallographic Society, Essen, Germany.
http://www.dgk-conference.de/

8-9 March 2018
SYNERGI2018. (SYnchrotron and NEutron Radiation Go Industrial, Amsterdam, Netherlands.
https://www.hzg.de/ms/synergi2018/070939/index.php.en

12-16 March 2018
ICDD Spring Meetings, Newtown Square, PA, USA.
http://www.icdd.com/profile/march18.htm

19-21 March 2018
3rd Annual Users Meeting of iNEXT, Grenoble, France.
http://www.esrf.eu/inext-annual-users-meeting-2018

19-23 March 2018
Muon Training Course 2018, Rutherford Appleton Laboratory.
https://www.isis.stfc.ac.uk/Pages/Muon-Training-Course-2018.aspx

20-23 March 2018
International Conference on Nanofilms 2018, Cranfield.
http://www.ecnf2018.org/

21-23 March 2018
4th 3D CLEM Conference, Ghent, Belgium.
https://corefacilities.vib.be/

21-24 March 2018
3rd International Symposium on Cryo-3D Image Analysis, Lake Tahoe, CA, USA.
http://cryoem.bcm.edu/cryoem/events/view_workshop/1

26-29 March 2018
BCA Spring Meeting, Warwick.
http://www.bcaspringmeetings.org.uk/

2-6 April 2018
2018 MRS Spring Meeting & Exhibit, Phoenix, AZ, USA.
http://www.mrs.org/spring2018

8-13 April 2018
Powder Diffraction & Rietveld Refinement School, Durham.
http://community.dur.ac.uk/john.evans/webpages/riet_register.htm

9-10 April 2018
Magnetism 2018, Manchester.
http://magnetism2018.iopconfs.org/home

11-12 April 2018
CCP-EM Spring Symposium, Keele.
http://www.cvent.com/d/9tq4ln

16-17 April 2018
The Astbury Conversation 2018, Leeds.
http://www.astburyconversation.leeds.ac.uk/index.php

24-27 April 2018
XOPT'18. International Conference on X-ray Optics and Applications 2018, Yokohama, Japan.
https://opicon.jp/info/20170601-876/

30 April – 4 May 2018
ICDD X-ray Fluorescence Clinic, Newtown Square, PA, USA.
http://www.icdd.com/education/xrf.htm

7-9 May 2018
15th Annual European Pharma Congress, Frankfurt, Germany.
https://europe.pharmaceuticalconferences.com/

12-19 May 2018
EMBO Practical Course on Characterization of macromolecular complexes by integrative structural biology, Grenoble, France.
http://meetings.embo.org/event/18-characterisation

13-17 May 2018
40th International Cement Microscopy Association (ICMA) Conference, Deerfield Beach, FL, USA.
https://cemmicro.org/annual-conference-information/

17-19 May 2018
7th Meeting 'X-ray and other techniques in investigations of the objects of cultural heritage', Krakow, Poland.
http://www.biurokarier.chemia.uj.edu.pl/conf/xray18

20-25 May 2018
12th New Diamond and Nano Carbons Conference (NDNC 2018), Flagstaff, AZ, USA.
http://www.mrs.org/ndnc-2018

20-26 May 2018
42nd International Symposium on Archaeometry ISA 2018, Merida, Mexico.
http://isa2018.mx/

21-25 May 2018
ISC2018. International School of Crystallization, Granada, Spain.
http://iscgranada.org/

27 May – 1 June 2018
Fatigue 2018, Poitiers, France.
https://www.sf2m.fr/Fatigue2018/Organization.htm

27 May – 1 June 2018
Les Houches/TSRC Workshop on Protein Dynamics, Chamonix Valley, France.
https://www.sites.google.com/site/houches2018/

1-10 June 2018
Electron Crystallography. 51st Erice Course, Erice, Italy.
http://crystalerice.org/2018/

1-10 June 2018
First Erice International School on Quantum Crystallography. 52nd Erice Course, Erice, Italy.
http://crystalerice.org/2018/

4-5 June 2018
Applied Crystallography, London.
http://crystallography.euroscicon.com/

4-8 June 2018
4D Workshop: Deep-time Data Driven Discovery and the Evolution of Earth, Washington, DC, USA.
http://www.4d-workshop.net

4-8 June 2018
Quasicrystals: pattern formation and aperiodic order, Edinburgh.
http://www.icms.org.uk/workshops/quasicrystals

4-8 June 2018
ICDD Clinic on X-ray Powder Diffraction: Session I – Fundamentals of X-ray Powder Diffraction, Newtown Square, PA, USA.
http://www.icdd.com/education/xrd.htm

6-8 June 2018
2nd Meeting on Porous Molecular Solids (PoMoS), Vietri sul Mare, Italy.
http://www.pomos.org/

10-14 June 2018
ISXB3. 3rd International Symposium on Halogen Bonding, Greenville, SC, USA.
http://isxb-3.org/

11-14 June 2018
55th Annual Meeting of the Clay Minerals Society, Urbana-Champaign, IL, USA.
http://conferences.illinois.edu/cms/

11-15 June 2018
ICDD Clinic on X-ray Powder Diffraction: Session II – Advanced Methods in X-ray Powder Diffraction, Newtown Square, PA, USA.
http://www.icdd.com/education/xrd.htm

11-16 June 2018
13th International Conference on Synchrotron Radiation Instrumentation (SRI 2018), Taipei, Taiwan.
http://sri2018.nsrrc.org.tw/site/page.aspx?pid=901&sid=1157&lang=en

13 June 2018
BCA Industrial Group XRF Meeting, Sheffield.
https://sites.google.com/site/bcaxrf/meetings/13-june-2018

18-19 June 2018
UK-Israel Summer School 2018 on NanoScale Crystallography for Bio and Materials, Tel-Aviv, Israel.
http://nano.tau.ac.il/Summer-School

18-21 June 2018
PCG Intensive School in Physical Crystallography: From Phonons to Phase Transitions
Cosener's House, Abingdon, Oxfordshire.
http://pcgschool2018.wordpress.com/

18-22 June 2018
2018 E-MRS Spring Meeting and Exhibit, Strasbourg, France.
https://www.european-mrs.com/meetings/2018-spring-meeting

18-26 June 2018
The 14th European Summer School on Scattering Methods Applied to Soft Condensed Matter, Carcans-Maubuisson, Gironde, France.
https://indico.ill.fr/indico/event/86/page/2

19-22 June 2018
MLZ Conference 2018 "Neutrons for Culture and Arts", Lenggries/Munich, Germany.
https://indico.frm2.tum.de/event/56/

24-28 June 2018
American Conference on Neutron Scattering (ACNS 2018), College Park, MD, USA.
http://www.mrs.org/acns-2018

24-29 June 2018
10th International Conference on the Occurrence, Properties, and Utilization of Natural Zeolites – Zeolite 2018, Krakow, Poland.
http://zeolite2018.org/

24-29 June 2018
Crystal Engineering (GRC), Newry, ME, USA.
https://www.grc.org/crystal-engineering-conference/2018/

25-27 June 2018
Science@FELs, Stockholm, Sweden.
https://indico.maxiv.lu.se/event/476/

25-28 June 2018
DSL2018. 14th International Conference on Diffusion in Solids and Liquids, Amsterdam, Netherlands.
http://www.dsl-conference.com/

26-29 June 2018
UKSR50. 50 years of Synchrotron Radiation in the UK and its global impact, Liverpool.
http://www.uksr50.org/

29 June – 1 July 2018
14th TOPAS Users Meeting, Edinburgh.
https://www.bruker.com/pt/events/users-meetings/x-ray-diffraction-and-elemental-analysis/topas-users-meeting.html

1-4 July 2018
EPDIC16 – The 16th European Powder Diffraction Conference, Edinburgh.
http://epdic16.efconference.co.uk/

2-6 July 2018
Combined Analysis in XRD by using MAUD software: 9th Workshop, Caen, France.
http://maud.radiographema.eu/

3-6 July 2018
Polarized Neutrons for Condensed Matter Investigations (PNCMI) 2018, Abingdon.
http://www.pncmi2018.org/home

8-13 July 2018
Aperiodic 2018, Ames, IA, USA.
https://register.extension.iastate.edu/aperiodic2018

8-13 July 2018
Geoanalysis 2018, Sydney, Australia.
http://ccfs.mq.edu.au/Geoanalysis2018/

8-13 July 2018
Sagamore2018, Halifax, Nova Scotia, Canada.
http://www.sagamore2018.ca/

9-13 July 2018
SIAM Conference on Mathematical Aspects of Materials Science, Portland, OR, USA.
http://siam.org/meetings/ms18/

11-13 July 2018
Methods and applications of crystal structure prediction: Faraday Discussion, Cambridge.
http://www.rsc.org/events/detail/24508/methods-and-applications-of-crystal-structure-prediction-faraday-discussion

20-24 July 2018
ACA 2018, Toronto, Canada.
http://www.amercrystalassn.org/2018-meeting-homepage

22-27 July 2018
XAFS2018. 17th International Conference on X-ray Absorption Fine Structure, Krakow, Poland.
http://www.xafs2018.com/

23-27 July 2018
18th International Conference on High Pressure in Semiconductor Physics (HPSP18) and Workshop on High Pressure Study on Superconducting (WHS2), Barcelona, Spain.
https://congresses.icmab.es/hpsp18-whs2/

23-28 July 2018
Particle based methods in materials science, Edinburgh.
http://www.icms.org.uk/workshops/particlebasedmethods

25-28 July 2018
χ-mag 2018, Nara, Japan.
http://www2.pe.osakafu-u.ac.jp/pe8/kai_mag2018/kai_magn2018_index.html

29 July – 3 August 2018
Diffraction Methods in Structural Biology (GRC), Lewiston, ME, USA.
https://www.grc.org/diffraction-methods-in-structural-biology-conference/2018/

5-9 August 2018
Microscopy & Microanalysis 2018 (M&M 2018), Baltimore, MD, USA.
https://www.microscopy.org/MandM/2018/

5-9 August 2018
ZMPC2018. International Symposium on Zeolites and Microporous Crystals, Yokohama, Japan.
http://www.jaz-online.org/ZMPC2018/

6-10 August 2018
Denver X-ray Conference, Westminster, CO, USA.
http://www.dxcicdd.com/

12-17 August 2018
Goldschmidt, Boston, MA, USA.
https://goldschmidt.info/2018/

13-17 August 2018
IMA XXII, Melbourne, Australia.
https://www.ima2018.com/

19-24 August 2018
XRM2018: 14th International Conference on X-ray Microscopy, Saskatoon, Saskatchewan, Canada.
http://xrm2018.com/

22-27 August 2018
31st European Crystallographic Meeting (ECM31), Oviedo, Spain.
http://ecm31.ecanews.org/en/index.php

26-30 August 2018
7th EuCheMS Chemistry Congress, Liverpool.
https://www.euchems2018.org/

27-30 August 2018
15th Biennial Meeting of the Society for Geology Applied to Mineral Deposits, Glasgow.
https://www.sga2019glasgow.com/

2-6 September 2018
SMARTER6, Ljubljana, Slovenia.
https://smarter6.ki.si/index.php/smarter6/

3-7 September 2018
XTOP2018. XIV Biennial Conference of High Resolution X-ray Diffraction and Imaging, Bari, Italy.
http://www.ba.ic.cnr.it/xtop2018/

9-14 September 2018
19th International Microscopy Congress. IMC19, Sydney, Australia.
http://imc19.com/

13-16 September 2018
ESCG2 Second European School on Crystal Growth, Varna, Bulgaria.
http://escg2.eu/

16-19 September 2018
8th Conference on Electron Tomography, Les Diablerets, Switzerland.
https://www.colorado.edu/symposium/etm2018/

16-20 September 2018
ECCG6 Sixth European Conference on Crystal Growth, Varna, Bulgaria.
http://eccg6.eu/

16-21 September 2018
SSC2018. 13th International Conference on Solid State Chemistry, Pardubice, Czech Republic.
http://www.ssc-conference.com/2018/

20-22 September 2018
HEC 21. 21st Heart of Europe Bio-Crystallography Meeting, Quedlinburg, Germany.
http://hec21.uni-halle.de/

22-25 September 2018
SEG2018. Metals, Minerals and Society, Keystone, CO, USA.
http://www.seg2018.org/

23-27 September 2018
Hot Topics in Contemporary Crystallography – HTCC, Bol (island of Brač), Croatia.
http://htcc2018.org/

24-28 September 2018
ICDD Rietveld Refinement & Indexing Workshop, Newtown Square, PA, USA.
http://www.icdd.com/education/rietveld-workshop.htm

7-12 October 2018
SAS2018. XVII International Conference on Small-Angle Scattering, Traverse City, MI, USA.
http://sas2018.anl.gov/

8-14 October 2018
ASMOSIA XII - Association for the Study of Marble & Other Stones in Antiquity XII, Izmir, Turkey.
http://asmosia2018.com/

16-19 October 2018
Neutrons and Food 5, Sydney, Australia.
http://www.ansto.gov.au/Events/Neutronsandfoodconference2018/index.htm

2-5 December 2018
AsCA 2018/Crystal32: 15th Conference of the Asian Crystallographic Association and 32nd Conference of the Society of Crystallographers in Australia and New Zealand (SCANZ), Auckland, New Zealand.
http://asca2018.org/

PCG Intensive School in Physical Crystallography

18th – 21st June 2018, Cosener's House, Abingdon

From Phonons to Phase Transitions:

- Translational Symmetry and Reciprocal Space - *Mike Glazer, Oxford*
- Phonons and Soft Mode Phase Transitions – *Martin Dove, QMUL*
- Irreducible Representation Analysis – *Mark Senn, Warwick*
- Landau Theory – *Michael Carpenter, Cambridge*
- Modulated Crystal Structures – *John Claridge, Liverpool*

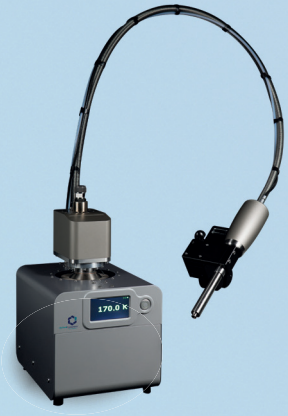
Registration is now open until the 12th of April 2018:

www.pcgschool2018.wordpress.com

British Crystallographic Association
XRF - INDUSTRIAL GROUP

The next XRF meeting is on Wednesday 13th June 2018 at Sheffield Hallam University.

This meeting offers a great opportunity for both novice and experienced users to enhance their XRF knowledge and discuss their requirements with major XRF suppliers in the exhibition. The morning has parallel sessions for Beginners and Experienced users and offers an ideal opportunity for anyone considering adding XRF to their analytical techniques. Attendees of these sessions will be given a certificate of attendance for their Continuing Professional Development.



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but you still have to make your own coffee

The new Smartstream is the optimal solution for small molecule crystallographers, offering 170 K (– 103° C) without liquid nitrogen.

Comprising a dry air supply and a combined cooler and controller, the **Smartstream** was designed to take in air and deliver a stream of gas at down to 170K. It really is that simple.

No liquid nitrogen, no cooling water, no 3-phase power supplies, no constant pumping.

The **Smartstream** was designed to do everything you need… except make the coffee, of course.

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