Crystallography News

British Crystallographic Association

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30th European Crystallographic Meeting in Basel

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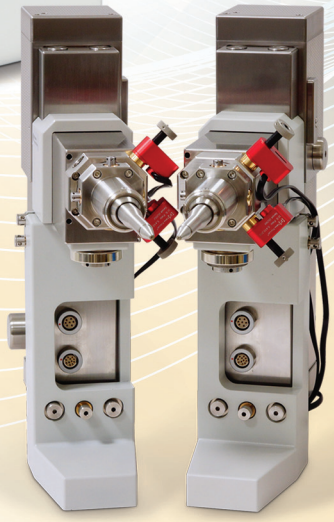

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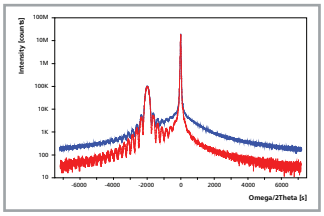

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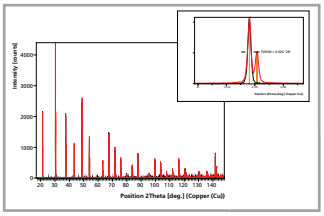

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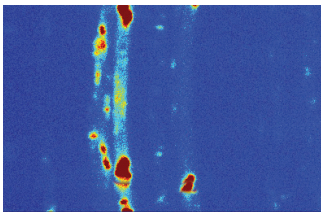

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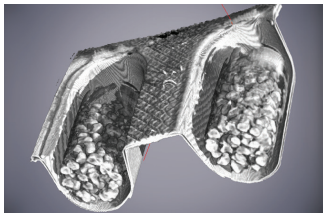

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CRYSTALLOGRAPHY NEWS is published quarterly (March, June, September and December) by the British Crystallographic Association, and printed by Bowmans, Leeds. Text should preferably be sent electronically as MSword documents (any version - .docx, .doc, .rtf or .txt files) or else on a PC disk. Diagrams and figures are most welcome, but please send them separately from text as .jpg, .gif, .tif, or .bmp files. Items may include technical articles, news about people (eg awards, honours, retirements etc), reports on past meetings of interest to crystallographers, notices of future meetings, historical reminiscences, letters to the editor, book, hardware or software reviews.
Please ensure that items for inclusion in the March 2017 issue are sent to the Editor to arrive before 25 January 2017.

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As required by the DATA PROTECTION ACT, the BCA is notifying members that we store your contact information on a computer database to simplify our administration.

These details are not divulged to any others without your permission. You may inspect your entry during the Annual Meeting, or otherwise by application to the BCA Administrative Office. We will be happy to amend entries at any time.

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This month's cover:

ECM30 opening session, dragon, the Rhine and Basel Zoo photographed by CHS and Elisa Nauha

From the President

IN writing this column, I looked back on where things were a year ago and find myself again on my annual visit to teach introductory solid state chemistry course in Nanjing, China. As I write we are in the midst of the autumn/winter meetings of the BCA groups, but can also look forward to the 2017 BCA meeting in Lancaster, the programme for is on track and can be found at http://www.bcaspringmeetings.org.uk/home. The deadline for submitted abstracts is 09.00 GMT, Friday 20th January, 2017.

In the latter part of the summer I put forward nominations for UK-based crystallographers to become members of 14 of the IUCr Commissions. I appreciate the willingness of those who were nominated to get involved and wish them luck in the selection/election process that takes places over the next year before being finalised at the IUCr General Assembly in Hyderabad next year.

The BCA Council held its autumn meeting in Sheffield in September. Among the key issues discussed were proposed changes to mechanism for selecting the award lectures and for identifying candidates for elected posts on BCA Council. Although the Early Career Awards, which now have an established symposium slot in the Spring Meeting programme, have mechanisms in place for nomination and selection of awardees, the process for the named lectures handled by the BCA (Dorothy Hodgkin Prize Lecture, Lonsdale Lecture, BCA Prize Lecture) have been a less formal process. The Bragg Lecture has always been chosen by the Bragg Committee, which is appointed by the Royal Institution. BCA Council have decided to put in place a nomination process for each of these lectures and to establish a three-year cycle of the Bragg, Hodgkin and BCA Prize lectures, with the Lonsdale Lecture being held annually. Further details are provided on page 10 of this issue. The Council also discussed the matter of nominations for elected positions on the Council, and specifically that there have been few contested elections in recent years. We are now considering the idea of establishing a Nominating Committee to ensure that BCA Members are presented with a choice of candidates for elections to the BCA Council. This move would follow the example and practice of other national crystallographic societies such as the ACA and SCANZ. We will be circulating a consultation document by email in December to encourage feedback which will help shape the proposal and determine if there is sufficient interest to bring it to the BCA AGM in 2017, along with any changes to BCA Statutes that would be required. No changes will take place for the 2017 elections and I will again encourage members to consider making nominations (or being nominated) for the post of Treasurer and that of Ordinary Member (replacing **Amber Thompson**), both of which will require election of new members of Council. Nominations should be sent to BCA Secretary **Claire Wilson** (secretary@crystallography.org.uk). The Council is also seeking someone to take on the role of webmaster for the BCA. Interested members should contact BCA VP **Richard Cooper** (richard.cooper@chem.ox.ac.uk).

The BCA will be launching a new Education and Outreach Programme to develop resources that can be used by the crystallographic community, teachers and community leaders for educational and outreach events. Funding will be made available to develop projects and to establish internships to develop resources. See the full announcement on page 10 of this issue.

In late September I attended the 24th annual meeting of the Croatian & Slovenian Crystallographic Association as one of their plenary speakers. The meeting was held in the coastal town of Bol on the island of Brač, off the coast from Split in southern Croatia. It was an enjoyable meeting in a very pleasant location. I was interested to see that the format of the meeting included no posters but there were a large number of talks from students, including many giving their first talk at a scientific meeting. This format is a regular feature if the meeting. This meeting was immediately followed in the same location by the 3rd European Crystallographic School, which included among its lecturers a number of UK regulars from the biennial BCA/CCG Intensive Teaching School in X-ray Structure Analysis: **Sandy Blake**, **Bill Clegg**, **Simon Parsons** and **Pete Wood**.

I would also like to note the recent death of Professor **Stanley C. Nyburg**, on September 2nd. Professor Nyburg was a noted crystallographer who spent significant periods of his long academic career in the UK and in Canada. Although I didn't know Stan personally, I was well acquainted with some of his work, particularly his early studies on short contacts between halogen atoms, which made use of the CSD and in which he discovered the now well-established polar-flattening, which has had an impact on my own long-standing interest in halogens and their involvement in hydrogen bonding and halogen bonding.

I'll close by repeating a call from my September column for any information that can enlighten me on crystallographic slide rules, a curiosity that I discovered at the Whipple Museum of the History of Science in Cambridge.

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BCA Council 2016

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(The dates in parentheses indicate the end of the term of office).

Full committee details on the BCA website

www.crystallography.org.uk

From the Editor

OUR big late summer event was the very successful European Crystallographic Meeting in Basel. On a previous visit to Basel Joan and I were delighted by its scenic location along the Rhine and impressed by the variety and quality of its museums. Therefore we chose to arrive a couple of days early so that we could spend the weekend before the conference sightseeing and enjoying the ambience. We did not reckon that Basel would become an outpost of the tropics during that weekend. With high temperatures both days around 35°C our will to sight-see evaporated, and we spent some considerable time just flopping down on a riverside bench in the shade watching the well-organised locals beat the heat in the inimitable Basel way. With a water temperature of 22°C and a swift current the Rhine provided the answer to overheating. The must-have item was a Wickelfisch: a large dry-bag in the shape of a round fish with a big tail. The sweltering Baselers would take a Rhine-side bus or tram to its upstream terminus, strip down to swimsuits putting clothing, personal possessions and a beach towel into their Wickelfisch, fold the tail over seven times and snap it shut. Holding on to their Wickelfisch, they would cast themselves into the current and enjoy the passing scenery until the sight of the harbour looming up ahead prompted a dignified exit up one of the flights of steps provided by the city, or an undignified scramble up the bank. The city had thoughtfully provided some portable changing rooms too, for swimmers to use when getting back into their street clothes; but with hundreds emerging from the water, the rooms were full. I had thought that Swiss people were reserved, but not here in the riverside parkland! With great skill they would form their beach towel into a cylinder around them, take off their wet swimwear and a bit later, like a caterpillar turning into a butterfly, emerge fully clothed.

As one would expect, the European Crystallographic Meeting was organised with Swiss precision. Particular credit for this goes to the Chair of the Organising Committee, Prof **Katharina Fromm** (University of Fribourg) and the Vice-Chair, Dr **Jürg Schefer** (Paul Scherrer Institute). At the Opening Ceremony Katharina complemented the speechifying with a convincing demonstration that she is a CHEMICAL crystallographer. As shown on the cover, her colleague Jürg held up a vessel in which a mixture that she had prepared reacted with a spectacular flash. We also enjoyed the sound of Swiss culture expressed in the mellow music of three alphorns. A legendary English presence in Basel is St. George's dragon. After being skewered by St. George on a tower of the Minster for several centuries, both are now well protected in the Museum Kleines Klingental. The scientific programme began and ended brilliantly with lectures by Nobel laureates **Ada Yonath** and **Jean-Marie Lehn**. I am grateful to **Elisa Nauha** and **Lilian Hayes** for reports on events at the conference which appear in this issue, and I also provide my own summary, which of course can only give patchy coverage of the wealth of information provided in the numerous parallel lectures. In case you wonder about the creatures on the cover photographed by Elisa, they were comfortably ensconced in Basel Zoo, which was the unusual venue for the conference dinner (and no, we didn't eat them, just admired them).

Several months earlier I had participated in another important European event, the well-attended annual meeting of the German Crystallographic Society in Stuttgart. My summary of some of the high points is included in this issue. Of course, there are meetings coming up that are much closer to home. Most of our Groups will already have held their Autumn Meetings by the time you read this, but there is still an opportunity to attend the Biological Structures Group Winter Meeting on Monday, 19 December at Birkbeck College in London. The topic is *"Seeing the Wood for the Trees in Structural Biology"*. Details are available on the BSG website. Be sure to get your skates on, as the closing date for registration is Friday 9 December. Structural biologists are in for a further treat early in the New Year. The CCP4 Study Weekend will take place from 9-11 January 2017 at Nottingham University.

The updated announcement in this issue will show that preparations are continuing well for the BCA Spring Meeting at Lancaster University from 10-13 April. Please note that the deadline for abstract submission is 09.00 Friday 20 January 2017, and Early Bird registration must be completed by Friday 10 March. As well as offering the usual fascinating science, this meeting is being held in a beautiful part of the country; and the slightly later date should give the balmy April breezes a good chance to penetrate to this northerly location. If you desire an even warmer atmosphere in which to enjoy exciting crystallography, you will get two opportunities: the ACA meeting in New Orleans 26-30 May (abstract deadline 15 February!) and the IUCr Congress in Hyderabad, India 21-28 August.

I write this column shortly after the announcement of the 2016 Nobel Prizes. The Chemistry prize was awarded jointly to **Jean-Pierre Sauvage**, **Fraser Stoddart** and **Bernard Feringa** "for the design and synthesis of molecular machines". Of course, if you want to construct any kind of machine, you need to think about its structure. If crystal structure determination is possible, it is the best way to verify the structure of a molecular machine or its components. I did a quick author search of the Cambridge Structural Database for these surnames (this could have been seriously misleading for Jones or Smith, but fortunately the surnames here are unusual), obtaining the following number of hits for each: Sauvage 133, Stoddart 761 and Feringa 177. Plainly, crystallography is very important to these authors, and we can once again take pride in our profession. You can read about their research at http://www.nobelprize.org/nobel_prizes/chemistry/laureates/2016/advanced-chemistryprize2016.pdf .

It only remains for me to wish you a happy holiday season and a happily untroubled crystallographic New Year of steady progress and success.

Carl Schwalbe

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The BCA values its close ties with commercial companies involved with crystallography. To enhance these contacts, the BCA offers Corporate Membership. Corporate Membership is available on an annual basis and includes the following benefits:

- Up to 10 free BCA memberships for your employees.
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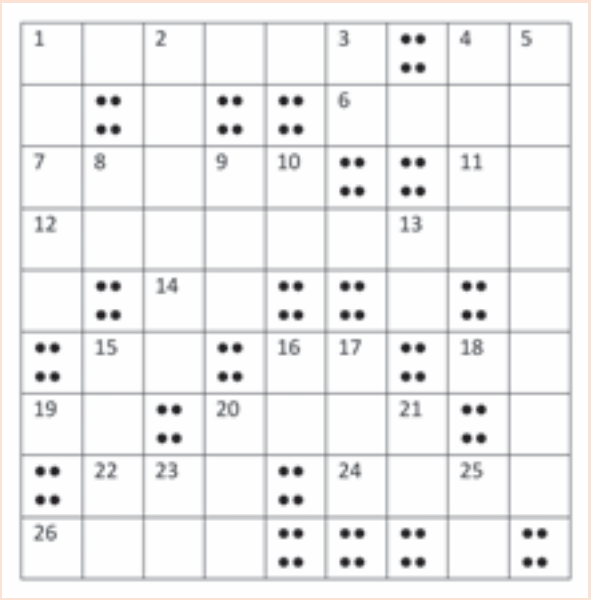
Puzzle Corner

THIS crossword puzzle has some seasonal references which I hope will get you into the holiday spirit.



Across

1. Continent drifting apart from the UK (6)
4. Element forming some crystalline clathrates, more common than the one in September CN (2)
6. Strong wind (4)
7. Bringer of seasonal gifts (5)
11. Found in all silicates (2)
12. X-rays, visible light, etc. (9)
14. Main power switch position required to generate 12 (2)
15. Morning time (2)
16. Naturally occurring element with the greatest density (2)
18. Element that recently formed its first crystalline clathrate, reported in September CN (2)
19. Symbol for 9 (2)
20, 22, 24. What you wish a Cockney or a smartphone on January 1 (4, 3, 4)
26. Where 7 has his headquarters (4)

Down

1. Bringer of scientific gifts (5)
2. Not systematic (6)
3. For example (1.1.)
4. In addition (4)
5. Animals that help 7 (8)
8. Hawaiian term for a type of basalt lava (2)
9. Element used for coating cans (3)
10. Hawaiian term for a type of basalt lava (2)
13. Type of 12 (2)
15. New year will be ???? Domini 2017 (4)
16. Short for a surgeon's work (2)
17. What children shouldn't do when 7 comes (3)
20. What we feel when contemplating a beautiful crystal structure like the ribosome (3)
21. God rest ?? merry gentlemen (2)
23. Short for an elevated railway (2)
25. Element used in aircraft (and a flying sleigh?) (2)

Answer to September Puzzle Corner on page 9

BCA Spring Meeting 10–13th April 2017

THE 2017 BCA Spring Meeting will take place at the University of Lancaster. The Young Crystallographers meeting starts at 13:00 on Monday 10th April and runs through to the morning of Tuesday 11th April. The YCG meeting is formally open to students and graduates within 5 years of their last degree, although all delegates are encouraged to attend. The main meeting starts with lunch and the first exhibitor's session at 12:15 on Tuesday 11th, and ends at 13:30 on Thursday 13th April.

Registration and abstract submission is now open at the meeting website: **http://www.bcaspringmeetings.org.uk/**

The deadline for online registration is Tuesday 4th April 2017, with Early Bird rates available until Friday 10th March 2017. A full residential package and day delegate packages are available. The deadline for abstract submission is Friday 20th January 2017. Abstracts will be reviewed by the Programme Committee after the abstract deadline and authors chosen for Oral and Poster presentation will be informed in early February.

We hope that you will contribute to make the meeting a success.

Andrew Bond
Programme Committee Chair

Scientific Programme

Monday 10 April, 2017

Young Crystallographers Group (YCG) Meeting

13:30–15:00 YCG Session 1
15:45–17:45 YCG Session 2
18:30–19:00 YCG Session 3: Flash Poster Presentations
19:00–21:00 YCG Poster Session and Buffet

Tuesday 11 April, 2017

08:45–11:15 YCG Session 4: How the Other Half Live

Main Meeting

11:30–12:15 **Lonsdale Lecture:**
Kay Diederichs (Universität Konstanz)
Towards a better understanding of (non) isomorphism in macromolecular crystallography

13:30–14:15 **CCG Plenary:**
Santiago Alvarez (Universitat de Barcelona)
Transition metal coordination polyhedra: shape, spin and secondary bonding

14:20–15:50 Extreme Conditions (PCG)
14:20–15:50 Computational Approaches (CCG)
14:20–15:50 Anti-Microbial Targets (BSG)
16:35–18:05 Order/Disorder (PCG)
16:35–18:05 Chemical Insights from Charge Density (CCG)
16:35–18:05 Extracellular Matrix and Cell Adhesion (BSG)

18:15–19:00 **PCG Plenary:**
Sharon Ashbrook (University of St. Andrews).
Investigating disorder and dynamics in solids using NMR spectroscopy

19:00–21:00 Poster Session and Buffet

Wednesday 12 April, 2017

08:45–09:30 **IG Plenary:**
David Rugg (Rolls Royce)
Crystallography for aerospace and nuclear sectors: an industrial perspective of the next decade

10:15–11:45 Phase Transitions (IG/CCG)
10:15–11:45 Complementary Techniques (CCG/PCG)
10:15–11:45 Multidisciplinary Protein Structural Analysis (BSG)
13:15–14:45 Early Career Researcher Prize Session
15:30–17:00 Crystallography of Minerals and Planets (PCG)
15:30–17:00 Multi-Component Crystals (CCG)
15:30–17:00 Advances and Challenges in Drug Discovery (BSG)

17:10–18:00 **Bragg Lecture:**
Mike Glazer (University of Oxford)
The wondrous world of perovskites

Thursday 13 April, 2017

08:45–09:30 **BSG Plenary:**
James Naismith (University of St. Andrews)
10:15–11:45 New Insights into Old Problems (PCG)
10:15–11:45 Extended Materials (CCG)
10:15–11:45 Tackling Cancer: New Approaches to Therapy (BSG)
12:00–13:30 Ad-hoc Session (PCG)
12:00–13:30 Would You Publish This? (CCG/YCG)
12:00–13:30 Multiprotein Complexes (BSG)

BCA 2017

Session Details:
Young Crystallographers Meeting

YCG Session 1
Chair: Claire Hobday (University of Edinburgh)
Plenary: Stefan Kaskel (Technische Universität Dresden)

YCG Session 2
Chair: Sam Horrell (University of Essex)
Plenary: Simon Coles (University of Southampton)

YCG Session 3:
Flash Poster Presentations
Chairs: Natalie Johnson (University of Newcastle), Alex Cousen (University of Bath)

YCG Session 4:
How the Other Half Live
Chair: Charlie McMonagle (University of Edinburgh)

Keynotes: **Matthias Gutmann** (ISIS), **Helen Playford** (ISIS), **Jane Endicott** (University of Newcastle)

This educational session aims to unite the fields of chemical, physical and biological crystallography. Three invited speakers will discuss their scientific approaches and point the way towards a brave new world of enlightenment and mutual understanding.

Session Details:
Main Meeting

Tuesday 11 April, 2017

14:20–15:50 Extreme Conditions (PCG)
Chair: Alex Gibbs (ISIS)

Keynote: **Stephen Blundell** (University of Oxford)

Working at extreme conditions can often provide critical access to particular areas of phase space and therefore deep insight into the behaviour of materials, along with surprises not predicted by current theory. The session will cover scientific and technological developments across a wide range of extreme experimental conditions such as high magnetic field, high temperature, low temperature and high pressure.

14:20–15:50 Computational Approaches (CCG)
Chairs: Anthony Reilly (CCDC), Krešo Bučar (UCL)

Keynote: **Colin Seaton** (University of Bradford)

The session will highlight computational methods in crystallography, crystal chemistry, materials science and crystal engineering. Emphasis will be on computational approaches aiding crystal-structure prediction and elucidation, structure-property correlations and predictions of physicochemical properties of organic, metal-organic and inorganic materials.

14:20–15:50 Anti-Microbial Targets (BSG)
Chair: Lydia Tabernero (University of Manchester)

Keynote: **Bill Hunter** (University of Dundee)

Infectious diseases are still a major health burden worldwide and the increase of antimicrobial resistance to current therapies poses a serious threat for their eradication. The session will focus on new targets and new approaches to tackle these important challenges.

16:35–18:05 Order/Disorder (PCG)
Chair: Helen Playford (ISIS)
Keynote: **Matthew Blunt** (UCL)

Structural disorder can be a material's defining feature. It can influence properties and applications, and change our understanding of fundamental physics. This session celebrates the order within disorder, with potential topics including (but not limited to): the structure of nanomaterials, single crystal diffuse scattering, pair distribution function analysis, self-assembly, low-dimensional materials, disordered magnetism, materials with anomalous physical properties, and so on. Studies that illustrate the challenges of dealing with complex materials are particularly welcome in this session.

16:35–18:05 Chemical Insights from Charge Density (CCG)
Chairs: Hazel Sparkes (University of Bristol), Graham Tizzard (University of Southampton)

Keynote: **Simon Parsons** (University of Edinburgh)

The session will examine approaches to obtain insights into chemical processes and properties through analysis of the electron density. The aim is to include results obtained using both experimental X-ray diffraction data and theoretical methods such as charge density analyses, Hirshfeld surfaces or PIXEL calculations to obtain a more detailed understanding of the charge distribution in the crystal structure.

16:35–18:05 Extracellular Matrix and Cell Adhesion (BSG)
Chair: Jordi Bella (University of Manchester)

Keynote: **David Hulmes** (CNRS, Lyon)

This session will focus on recent developments on the structural biology of extracellular matrix proteins and cell adhesion molecules including crystallographic analysis of their biosynthesis and molecular assembly mechanisms, processing, secretion and extracellular matrix deposition, and cell-extracellular matrix interactions.

Wednesday 12 April, 2017

10:15–11:45 Phase Transitions (IG/CCG)
Chair: Tony Bell (Sheffield Hallam University; IG), Katharina Edkins (University of Durham; CCG)

Keynote: **Quanshun Luo** (Sheffield Hallam University)

The session will discuss phase transformations, including characterisation techniques and associated modelling. The aim is to discuss a broad range of chemical and materials systems under a variety of environmental conditions. Relevant abstracts are invited from all areas of the community.

10:15–11:45 Complementary Techniques (CCG/PCG)
Chairs: Elliot Carrington (University of Sheffield; CCG), Emma McCabe (University of Kent; PCG)

Keynote: **Paul Hodgkinson** (University of Durham)

Significant developments have recently been made to characterise crystalline and non-crystalline materials using techniques other than diffraction. Such methods are often

especially valuable for materials whose behaviour is affected by local structure or disorder. The session will focus on complementary characterisation methods such as spectroscopy, and insights from theory and physical properties, including work from both chemical and physical crystallography backgrounds.

10:15–11:45 Multidisciplinary Protein Structural Analysis (BSG)
Chair: Clair Baldock (University of Manchester)

Keynote: To be confirmed

Understanding the structure-function relationships of complex biological systems usually requires data obtained from several structural techniques that provide complementary insight into the biological problem. This session will look at recent developments on the combination of crystallographic analysis with techniques such as small angle X-ray scattering, NMR, electron microscopy or electron paramagnetic resonance, amongst others.

15:30–17:00 Crystallography of Minerals and Planets (PCG)
Chair: Anthony Phillips (Queen Mary)

Keynote: **Simon Redfern** (University of Cambridge)

Crystals are ubiquitous throughout our world and beyond it; we will focus in this session on the many applications of crystallography to Earth and planetary science. This might include experimental and computational studies of structure under geological conditions, at extremes of temperature and pressure; analysis of minerals with terrestrial or extra-terrestrial origins; and even remote crystallography from space missions.

15:30–17:00 Multi-Component Crystals (CCG)
Chairs: Gareth Lloyd and Hayley Green (Heriot-Watt University)

Keynote: **Krešo Bučar** (UCL)

The session aims to highlight research on multi-component crystalline systems including co-crystals, solvates, hydrates, and inclusion compounds. Of particular interest is understanding structure-property relationships in such materials through their design and characterisation.

15.30–17.00 Advances and Challenges in Drug Discovery (BSG)
Chair: To be confirmed

Keynote: **Rod Hubbard** (University of York)

Recent years have brought the development of different approaches in drug development leading to more specific and sophisticated targeted therapies. Structure-based fragment methodologies together with protein-protein interaction inhibitors are now generating new opportunities for drug development. The session will focus on new advances and challenges in drug discovery and how structural analyses support their development.

Thursday 13 April, 2017

10:15–11:45 New Insights into Old Problems (PCG)
Chair: Mark Senn (University of Oxford)

Keynote: **Abbie McLaughlin** (University of Aberdeen)

The session aims to present work that brings new structural insights into long-standing problems, where new methodology or unconventional techniques have been used to tackle problems which have conventionally been viewed as insoluble or, where the study of new materials has led to old problems being re-evaluated. Abstract submission is encouraged from a broad range of scientific areas.

10:15–11:45 Extended Materials (CCG)
Chairs: Helena Shepherd (University of Kent), Jonathan Foster (University of Sheffield)

Keynote: **Neil Champness** (University of Nottingham)

Designing and synthesising extended materials with a desired topology remains an outstanding challenge in crystal engineering. Understanding how to control the assembly, and ultimately the properties, of such materials requires insights from a wide range of techniques alongside crystallography. The session welcomes contributions from speakers working with a diverse range of materials.

10:15–11:45 Tackling Cancer New Approaches to Therapy (BSG)
Chair: To be confirmed

Keynote: **Jane Endicott** (University of Newcastle)

Cancer is a multifactorial complex set of diseases that respond to a number of environmental and intrinsic factors. Understanding the molecular basis of different types of cancer is essential to progress towards better treatments. The session will focus on new potential targets for cancer therapy as well as recent advances on the development of protein inhibitors of known targets.

12:00–13:30 Ad-hoc Session (PCG)
This session is set aside to encourage presentation of the latest results that may not fit within the other session topics. Abstracts are invited from any area of physical crystallography.

12:00–13:30 Would You Publish This? (CCG/YCG)
Chairs: William Lewis (University of Nottingham; CCG), Claire Hobday (University of Edinburgh; YCG)

Keynote: **Iñigo J. Vitórica-Yrezábal** (University of Manchester)

This interactive session will discuss problematic crystal structures that can be hard to interpret and publish. After the opening keynote talk, the session is open for anyone to describe structural results that raise the session title question. The audience will discuss, with the aim to provide constructive advice. Problems might include charge imbalance or other chemical issues, poor resolution or data completeness, complicated disorder, highly restrained models, unexplained residual electron density, etc. A formal abstract is not required, but please contact the session organisers in advance of the meeting (as soon as possible!) if you wish to contribute; 1-3 slides will be requested for concatenation into a single session presentation. Contributions from YCG members are particularly encouraged.

12:00–13:30 Multiprotein Complexes (BSG)
Chair: Steve Prince (University of Manchester)

Keynote: **Mark Banfield** (John Innes Centre)

Multiprotein complex formation is at the centre of critical biological processes such as macromolecular assembly, receptor-ligand recognition, or host-pathogen interactions. Crystallographic analysis of these complexes remains a challenging problem due to technical complexity that starts at the molecular biology level and extends all the way to the structure determination. This session will look at recent representative examples of crystallographic analyses of multiprotein complexes, the difficulties encountered, and the approaches taken to overcome them.

Programme Committee

Chair: **Andrew Bond** (University of Cambridge).

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

BSG: **Lydia Tabernero** (University of Manchester), **Jordi Bella** (University of Manchester).

CCG: **Gareth Lloyd** (Heriot-Watt University), **William Lewis** (University of Nottingham).

IG: **Ghazala Sadiq** (CCDC), **Helen Blade** (AstraZeneca)

PCG: **Nick Funnell** (ISIS), **Jan-Willem Bos** (Heriot-Watt University).

YCG: **Sam Horrell** (University of Essex), **Claire Hobday** (University of Edinburgh).

Workshops: **Horst Puschmann** (OlexSYS).

Organisers: **Joanne McBratney**, **Nicola Peel** (Hg3 Conferences).

Answer to September Puzzle

In order of appearance:

1. At high temperatures thymine monohydrate ejects water.
2. The cavitand has been used for the enclathration of over 20 small gases. Release from the clathrate has been studied for water, nitrogen, carbon dioxide, krypton and fluoromethane.
3. The specially designed porous material can capture acetylene from acetylene/ethylene mixtures with the acetylene to undergo desorption later.
4. The multidrug transporter EmrD from *Escherichia coli* expels amphipathic compounds across the inner membrane.
5. The multidrug ABC transporter Sav1866 from *Staphylococcus aureus* binds ATP, making the transmembrane domains face outward to export a variety of cytotoxic drugs.

BCA Announcements

Applications sought to develop Education and Outreach resources in Crystallography for reuse within and beyond the crystallographic community

THE BCA has established a fund to provide support to develop education and outreach activities and resources that enable others to run events. This goal will be realised through two routes and we are seeking applications from BCA members to contribute towards its development.

1) **Development of resources to support Outreach activities.** These can range from physical materials made available via the inventory (see below) or electronic resources such as downloadable activity packs, guidance materials for conducting an exercise or software applications. These can be applicable to any age group or audience, i.e. school teachers or scout/guide leaders are as relevant as academics! It is expected that the funding is for the development of openly available resources so that they can be reused by anyone, although trialing and evaluating them at specific outreach events as part of a funded project is perfectly acceptable.

2) **Enhancements to the learn.crystallography.org.uk site to support Outreach activities.** Although we are receptive to new ideas, we will prioritise work in the following areas: an open repository of electronic materials for supporting Outreach activities; the development of an online inventory of outreach resources with capability for an individual to book out physical items; a system for anyone to register an Outreach event in a public calendar and be able to make a call to subscribers for volunteer help to conduct the activity.

Funding is available at two levels. Support may be sought for 8-week internships to fund undergraduate students to develop resources – these would normally be up to a level of £2500 for a stipend and materials. Alternatively, an individual may request funds of the order of £300 to purchase materials required to develop an activity. These costings are indicative only and a funding breakdown summary will be required as part of the application.

Applications from Early Career Researchers are particularly favoured, either to perform the work or to supervise an intern. However, a supporting statement is required from a supervisor to indicate that the appropriate environment to conduct the work will be provided.

Applications or enquiries should be emailed to **Simon Coles** (s.j.coles@soton.ac.uk) and the closing date for the 2017 round will be 17:00 on Friday 3rd March 2017. Applications will be reviewed by the Education Committee (comprising the Education and Outreach Coordinator and the education representatives from the BCA groups) and potentially in some cases also by BCA Council.

Before making any award the committee may approach you for further clarification. It is expected that an annual call for internships will be made around the end of the calendar year, although in exceptional circumstances applications may be submitted outside of this timeframe after prior communication with the Education and Outreach Coordinator. The committee will seek to balance these activities across the remits of all the BCA Groups. The Terms and Conditions of these bursary awards will be published on the BCA website.

Call for Nominations for BCA Named Lectures

THE BCA awards and hosts a number of named lectures at its annual Spring Meeting. These lectures have been presented to date on a semi-regular basis, but following a decision by BCA Council will henceforth be presented on a regular schedule. The Dorothy Hodgkin Prize, The Bragg Lecture, and The BCA Prize Lecture will each be awarded once in a 3-year cycle. The Lonsdale Lecture, presented at the interface between YCG and main meetings, and The Parkin Lecture, presented during the YCG Satellite Meeting, will be awarded annually. Details of each award and previous winners are available on the BCA website crystallography.org.uk/prizes/.

The Parkin Lecture, 2017

Nominations are sought for the Parkin Lecture, due to be presented at the 2017 BCA Spring Meeting. The Parkin Lecture is awarded by the Young Crystallographers Group of the BCA. This lecture is named in memory of the late Dr Andrew Parkin and recognises his outstanding achievements as scientist and teacher, and his role in public outreach. Nominations of early career scientists who have had significant involvement in teaching and outreach activities should be submitted by email to the YCG chair (shorrell@essex.ac.uk) with a short (< 250 words) case for support. The deadline for nominations is February 1st 2017.

The Dorothy Hodgkin Prize Lecture, 2018

Nominations are sought for The Dorothy Hodgkin Prize Lecture, due to be presented at the 2018 BCA Spring Meeting. Awardees generally work in an area of crystallography in which Dorothy had an interest, but nominations are welcomed from any part of the crystallographic community.
Submissions should be sent by email to the BCA President (president@crystallography.org.uk) and include a short (< 500 words) case supporting the nomination. The deadline for nominations is February 24th 2017.

The Lonsdale Lecture, 2018

Nominations are sought for The Lonsdale Lecture, due to be presented at the 2018 BCA Spring Meeting. The Lonsdale Lecture is awarded by the BCA on the recommendation of the Young Crystallographers Group. The range of topics that may be presented by the awardee encompasses all areas of crystallography and diffraction and the lecture is expected to have an element of teaching. Nominations for The Lonsdale Lecture should be sent to by email to the BCA President (president@crystallography.org.uk) and include a short (< 500 words) case supporting the nomination. Awards are made in consultation with and upon the recommendation of the Young Crystallographers Group. The deadline for nominations is February 24th 2017.

Draft minutes of the BCA Annual General Meeting 2016

6pm April 6th, room B52, Business School South, Jubilee Campus, University of Nottingham

1. **Approval of the agenda –** with elections brought forward prior to President's report
   Proposed by Pamela Williams and *seconded by Mike Probert* and approved by the meeting.

2. **Apologies for absence –** none received.

3. **Minutes of the AGM 2015.**
   The minutes had been circulated previously by email, are available in the members area of the BCA website and had been published in *Crystallography News* March 2016 edition. *Proposer Mike Glazer*, *seconded by Jeremy Cockcroft and accepted without corrections.* The President updated the meeting that Mike Glazer, Vice President of the IUCr had brought up the issue of costs of adherence to the IUCr with the IUCr and discussions are underway.

4. **Elections to Council (brought forward from item 10).**
   The following candidates had been nominated: for Vice-President – *Richard Cooper (nominated by Paul Raithby, seconded by Iain Oswald)* and *Jeremy Cockcroft (nominated by Judith Howard and seconded by Paul Barnes)*; for *Secretary Claire Wilson (nominated by Simon Parsons and seconded by Ivana Evans)* and for Ordinary Council Member *Anna Warren (nominated by Claire Wilson and seconded by Elizabeth Shotton)*. Both candidates for Vice-President gave a short speech and votes were cast by a secret ballot of the members of the BCA. Richard Cooper was re-elected as Vice-President. Claire Wilson (Secretary) and Anna Warren (Ordinary Council member) were elected unopposed by a show a hands. Jeremy Cockroft was thanked for standing for Vice-President.

   It was highlighted that elections will be held in 2017 for the Treasurer and for a further ordinary council member, who would normally be from the CCG to maintain balance on council.

5. **President's report**
   The President noted several crystallographers who had passed away in the last year: Dennis S. Beard, Norman A. Curry and Eric J.W. Whittaker and he thanked colleagues who had written obituaries for *Crystallography News*.

   Spring Meeting 2016: The President thanked Phil Lightfoot, the programme chair for being tremendous in organising the meeting and being very easy to work with, Richard Cooper, Vice-President and point of contact with Council, Nicola Peel and her colleagues at Hg3, and noted appreciation for everyone's contribution to an excellent meeting.

   Spring Meeting 2017: This will be held in Lancaster and Andrew Bond (University of Cambridge) has agreed to be programme chair. The planning will begin at this meeting with an initial brief meeting of the members of the 2017 programme committee on Thursday. The main planning meeting will take place in late May or early June which is a little earlier than usual to give more time. The President encouraged everyone to put forward suggestions for symposia or plenary speakers to their group reps.

   The President congratulated John Helliwell on being presented with the 8th Max Perutz award at the ECM in 2015 and Elspeth Garman who is the recipient of the ACA Fankuchen Award for 2016. He noted that these are both major awards and it's good to see British Crystallography being acknowledged around the world.

   The President reflected on a couple of important celebratory events that took place in the last year. The CCDC 50th anniversary CSD50, July 1st-3rd, 2015 opened by Olga Kennard and closed by Colin Groom, was a fantastic event. Judith Howard's career celebration symposium took place on September 17th, 2015, in Durham. It was organised by former students and other collaborators who managed to keep it a surprise for Judith.

   Education and Outreach was reported on, with slides provided by Simon Coles, Education and Outreach coordinator. Events that took place included Cheltenham Science festival in the Warwick 'What if' tent. Thanks were given to Pam Thomas and her team, in particular Mike Glazer and Jonny Brooks-Bartlett. A number of other events were highlighted, for example, Michael Wharmby at Diamond organised events at the 25th Orkney International Science Festival; Lynne Thomas (Bath) participated in Soapbox Science – an event with female scientists on a box in Bristol for an hour talking to the public; YorNight; European researchers night in York and National Science and engineering week family day at Southampton. The BCA did not participate in the Big Bang Fair this year due to a number of partners deciding not to attend. This prompted a review of how the BCA is involved in future events, how we develop resources and infrastructure, both physical and electronic, that allow BCA members to be involved in events. The intention is to have a stand that anyone can use, a 'central library' of resources to support outreach and development of the learn.crystallography.org.uk site to be a central repository for electronic resources and provide a place for members to register an event and call on volunteer helpers if necessary. Simon Coles has been talking with Diamond and ISIS outreach teams to better align with them and operate collaboratively. Internships have been proposed to council and agreed in principle to provide modest funding to develop learn.crystallography.org.uk further and generate new outreach resources that can be used by all. Contact details for the EOC Simon Coles and the

group EOC reps were given; BSG Jacob Butler (Cambridge), CCG Graham Tizzard (Southampton), PCG Mike Glazer (Oxford), IG Ghazala Sadiq (CCDC) and YCG Jonny Brooks-Bartlett (Oxford).

The President concluded his report with thoughts on priorities for the BCA going forward; a continued focus on the strength of the Spring Meeting, the quality and diversity of science, opportunities for presentations at all career stages. It has been a very good meeting with good attendance. We need to continue to focus on the financial health of the BCA and to develop Education and Outreach activities. The BCA website is an important communication tool and the President was keen to hear from members about the content, what's missing and what should be added.

6. **Secretary's report –** no report given, questions welcomed.

7. **Hg3 report.**
Nicola Peel reported 258 registrations (250 in 2015) with the following breakdown for the main meeting; full residential package 173, day delegate 56 and exhibitors 16 with 118 delegates for the YCG satellite. The group breakdown by group was 57 BSG, 118 CCG, 14 IG, 51 PCG. The full residential package model this year was much simpler.

Membership figures were also reported with a total membership of 740 at March 31st 2016. The corporate members were named; Bruker UK, Cambridge Crystallographic Data Centre, Douglas Instruments Ltd, International Centre for Diffraction Data, Incoatec GmbH, Molecular Dimensions Ltd, Oxford Cryosystmes Ltd, Panalytical Ltd, Rigaku Oxford Diffraction and thanked very much for their support.

Crystallography News has slightly fewer advertisers.

8. **Treasurer's report**
The Treasurer reminded members that the accounts report on the period from Jan 1st 2015 to Dec 31st 2015. A more detailed breakdown is in the summary financial statements which were handed out and a full breakdown is included in the BCA annual accounts, available by email or online at the Charity Commission website.

It was noted that the large changes in income from meetings of the groups in alternate years is due to the CCG Intensive School which runs every other year. In general the finances are stable and the governance expenses kept stable and the aim is to keep these low, allowing the award of bursaries and spending on outreach to continue.

The Spring Meeting in York in 2015 made a slight loss but an improvement on the 2014 meeting in Loughborough. Venues have a particular cost and the budget is set to try to break even.

Significant outgoings are for the subscriptions to the IUCr and ECA and the spring meeting. *CN* continues to bring in income as does the CCG school.

The Treasurer summarised her report by stating that we continue to try and reduce our governance costs and maintain a cautious, balanced investment of funds. Overall BCA total income rose slightly last year compared to previous years (£248,720 compared to £244,744 in 2014) and we continue to award bursaries and sponsor outreach activities. She concluded with thanks to Hg3, BCA Council members, SIG treasurers, Charles Stanley Bank and the Young Company accountants.

John Helliwell asked whether Council had a more optimistic view this year than last year concerning the future income of the BCA and IUCr subscriptions. The Treasurer replied that it had been important to have the discussion so that the membership was aware of the situation and with the increased membership fees we will be able to hold a stable position rather than depleting funds, allowing us to continue to support bursaries and outreach activities. The President commented that the discussion last year at the AGM was very valuable and a clear message had been given by the membership and Council had acted accordingly. Pierre Rizkallah asked if the increased membership was in the accounts presented and it was clarified that the increase was for 2016 fees and would appear in this year's accounts.

9. The accounts were accepted, *proposed by Pierre Rizkallah and seconded by Jeremy Cockcroft*.

10. The Young Company were appointed as the examining accountant for 2016, fee £5100, *proposed by Mike Probert and seconded by Dave Keen*.

11. **Honorary members**
Honorary members are chosen for their contributions both to crystallography and to the BCA and retain their membership for life. The number of honorary members at any one time is limited as is the number added in a particular year. Honorary members may be proposed by any member by sending a recommendation to the President, ideally supported by others and the President encouraged the members to make nominations for this important award.

Two nominations for new honorary members were approved this year: Eleanor Dodson, FRS and Olga Kennard, FRS, both very well known crystallographers who have made significant contributions to the field of crystallography over a long period of time and the President said he was very pleased to award these honorary memberships.

12. **Membership, annual subscriptions and subventions**
A breakdown of the membership numbers by group was given for the end of year 2014 and 2015 showing an increase from 638 total members to 666 in 2015. The membership fees for 2016, as approved at the 2015 AGM, are £35 full membership, £17.50 concessions, £58.50 student (4 years) and £175 overseas members (5 years). A straw poll at the 2015 AGM indicated that there was support to further increase fees but it was decided that was not necessary this year although it is likely that it will be returned to in the near future.

13. **AOB**
Simon Parsons commented that there was a large increase in YCG membership, from 44 (2014) to 128 (2015). Sam Horrell clarified that although there is an increase the figures also reflect that this information is now captured by Hg3, whereas previously it was only membership of the 4 groups BSG, CCG, PCG and IG.

A comprehensive thank you was given to everyone involved in organising the meeting.

The AGM closed at 19:00.

ECM30

THE statistics presented at the welcome session demonstrated that this meeting was highly successful. It attracted 920 participants from 47 countries. The extensive scientific coverage included 2 plenary lectures, 16 keynote lectures, 50 microsymposia and around 400 posters. Leading nations in terms of abstract submissions were Switzerland (103), Germany (95) and the United Kingdom (71). In a series of beautifully articulate and concise welcoming speeches, a presentation by Joel Mesot (Paul Scherrer Institute, PSI) presented some information about the PSI that will be of interest to many of us. The PSI welcomes about 2500 visitors per year, approximately 50% from Switzerland, 40% from the European Union and 10% from elsewhere. Over 11% of synchrotron and around 5% of neutron beam time is sold to industry. Its free electron laser is expected to produce its first beam on December 5 and will attain brilliance 10^{10} times higher than that of a synchrotron. The first evening culminated with the Perutz Prize lecture. This year's winner was Dr. Václav Petříček (Czech Academy of Sciences), honoured for practical application of the theory of aperiodic structures in the development of the program JANA over 3 decades. It can now be used in the analysis of incommensurate, commensurate and composite structures from single crystal and powder X-ray as well as electron diffraction data. Sometimes three dimensions do not suffice to describe a structure. An early example was the appearance of satellite spots (Gittergeister, "lattice ghosts") in the diffraction pattern of sodium carbonate noted in 1927. While in a classical crystal all diffraction spots can be indexed by a reciprocal vector h = ha' +kb' + lc', here an extra term mq had to be added, where q was generally incommensurate with the reciprocal lattice vectors a', b', c'. This modulated structure becomes periodic in 4 dimensions. Superspace theory won the Ewald Prize in 2014. The latest version of JANA can go up to 6 dimensions and can handle merohedric, reticular and pseudo-merohedric twinning as well as modulated magnetic structures.

Monday got off to a spectacular start with the lecture by **Ada Yonath** on crystallography and ribosomes. Plainly she has not been resting on her Nobel laurels. Mammalian cells may contain millions of ribosomes (5-6 million in the case of liver cells) which can make up to 40 peptide bonds per second in the biosynthesis of proteins. Pathogenic organisms have ribosomes too, and >40% of clinically used antibiotics disable protein biosynthesis. A YouTube video illustrating the action on the ribosome of disparate classes of antibiotics is available at https://www.youtube.com/watch?v=RedO6rLNQ2o . As with all antibiotics, resistance is a growing problem with ribosome-blocking antibiotics. Ada and her colleagues have been examining the structures of ribosomes from resistant pathogens such as *Staphylococcus aureus*. Pleuromutilins are a promising class of antibiotics that inhibit protein synthesis in this pathogen among others. A crystallographic study by Ada and colleagues using synchrotron radiation showed where on the ribosome this class of drugs binds, and she is working with a pharmaceutical company to discover improved analogues. Desirable properties include enhanced specificity, to safeguard not just host cells but also beneficial micro-organisms. Universal conservation of the ribosome core has implications for the origin of life.

MS10 covered hydrogen bonding and weak interactions in crystals. **Heloisa Bordallo** told us about nanoscale hydrogen bond networks revealed by neutron scattering. Unexpected differences in N-D bond lengths in D- and L-alanine were revealed by neutron powder diffraction. Polymorphs of paracetamol differ in their layers: stable form I makes corrugated layers while metastable form II has flat layers which facilitate cohesion under direct compression. The weaker hydrogen bond network in II is enhanced at high pressure, and this form becomes stable. **Katharina Edkins** continued the discussion of molecular interactions in pharmaceutical compounds. Theophylline can form crystals both as a hydrate and as an anhydrate. Understanding the role of water in the crystal is essential to explain the lower solubility of the hydrate. Furthermore, heating anhydrate Form I to 232°C converts it to Form II, which also results from holding the monohydrate at low humidity. The monohydrate gives tiny crystals with 50:50 disorder of water, located in channels. Solvates may also have altered charge distribution. Piroxicam is neutral in forms I, II and III but a zwitterion in its hydrate. **Alberto Podjarny** applied high-resolution X-ray (to 0.98 Å) and neutron (to 1.90 Å) protein crystallography to probe the large internal cavity in heart fatty acid binding protein (H-FABP) complexed with oleic acid. The cavity contains the oleic acid and also a mainly tetrahedric cluster of water molecules. The preferred alignment of water molecules reduces the effective dielectric constant from ≈80 to ≈20, enhancing long-range electrostatic forces. **Ai Woon Yee** also combined neutron with X-ray proton crystallography. The transport protein transthyretin normally exists as a homotetramer formed from a dimer of dimers. In crystals the dimer is the asymmetric unit. Unfortunately, if the tetramer dissociates to release monomers, they may mis-assemble into fibrils leading to amyloid disease. Mutations can affect the stability of the tetramer: S52P readily forms amyloid while T119M is super-stable and avoids creating amyloid. Deuteration of S52P and quasi-Laue neutron diffraction to resolution 1.8 Å enabled high-resolution structure determination. Back exchange from D to H revealed regions of instability. The monomer-monomer interface is stable, but backbone residues 69-72 show back exchange in S52P but not wild type. **John Wallis** concluded the session with analysis of *peri*-substituted naphthalenes. If the substituents at positions adjacent to the bridge are a dimethylamino group and an alkene, attractive interactions between them or even bond formation ensue. Charge density measurements and the "Atoms in Molecules" approach facilitate the monitoring of progress to bonding. An aldehyde group instead of the alkene can be protonated at O with incipient N-C bond formation. With three ketones protonation leads to N-C bonds ≈1.66 Å. With a carboxylate group adjacent to an aldehyde an OCO^{-}…C-O distance around 2.6 Å may develop.

In her Keynote Lecture **Francesca Fabbiani** explored crystalline molecular interactions at high pressure. The Cambridge Structural Database (CSD) contains 1502 entries for high-pressure studies between 1971 and 2015. The first one was C_6H_5Cl by Roger Fourme in 1971. A chloroform study demonstrated the need for overpressurisation due to the "laziness" of crystallization. Crystals may be prepared at high P by direct compression of existing crystals, growth from melt or growth from solution. People who report new phases may fail to provide vitally important information about the synthesis protocol. A substance that survives direct compression without crystal damage is vitamin B12. At ambient pressure about 33% of the crystal volume is water, disordered in channels and ordered in pockets. Above 1 GPa a conformational switch occurs and water in channels becomes ordered. Use of high pressure is not yet routine in polymorph screening, even though the applied load during tableting is 40-200 MPa (sometimes 400). GABA monohydrate has been crystallized from 6-12 M aqueous solution at 0.4-0.8 MPa, where the hydration enthalpy of -5 to -9 kJ mol^{-1} has been determined, compared with near zero at ambient pressure. Denser polymorphs are expected to be more stable at high pressure.

The Bertaut Prize was awarded to **Linda Reinhard**, whose prize lecture had the title "Solving problems leads to solving crystal structures". A homogeneous sample is the most important thing for good protein crystallization. Then it becomes necessary to find the protein's comfort zone, in terms of pH, ionic strength, temperature, etc. The buffer can be optimised by reference to thermal stability. The principle of Thermofluor is that folded protein + dye gives no fluorescence while unfolded protein exposes hydrophobic patches to which dye adsorbs and can fluoresce. Thus the temperature at which the protein unfolds can be determined, allowing the buffer that gives the highest unfolding point to be identified. Controlled dehydration can sometimes be useful. After mother liquor has been removed from around the crystal, controlled humidity air is passed over it, followed by freezing and testing. A current project is RNAse P. The active site has been found to be disordered, prompting some questions. Is this disorder physiological or a crystallization artefact? Does it arise because other components have been removed?

The next morning **Simon Parsons** gave a thought-provoking lecture on "Understanding the driving forces of phase transitions in molecules" (spelled "diving forces" in the Programme Booklet). We have acquired some hard-won understanding of internal energy U and its components such as electrostatic, dispersion, polarisation and repulsion. However, Simon reminded us that it is the Gibbs free energy G = U + pV – TS which governs stability, not just the energy U. For example, a volume decrease of 7 $Å^3$ at a pressure of 5.3 GPa lowers the free energy by 23 kJ mol^{-1}, which is very significant, and the entropy term can make a difference as well. Amino acids studied up to 10 GPa include glycine, serine and methionine. The unit cell volume of serine decreases smoothly as pressure rises to 5 GPa but then drops sharply because of a phase change. Likewise, the N…H-O distance decreases gradually to 2.69 Å, but it jumps to > 2.8 Å at the phase change as hydrogen bonded rings collapse. Since this collapse fills voids, pΔV is large and negative. In the region up to 10 GPa contacts seem to be driven to minimum values found in the CSD but almost never become super-short. The polymorphism of glycine is instructive. Under ambient conditions the γ form is most stable, but at high pressure conversion to ε occurs. For the change γ to ε ΔV is -1.5 $Å^3$, corresponding to -0.5 kJ mol^{-1} at 0.5 GPa. Full interaction maps show that in the γ form the ammonium and carboxylate groups are positioned exactly where they would be expected, but in ε some blobs are unfilled. PIXEL calculations indicate that some N-H…O contacts are repulsive, not because of the hydrogen bond itself but because two NH_3^+ groups are brought too close together. Simon's conclusion is that a focus on contact distances can be misleading, and one must consider whole-molecule interaction energies.

MS30 continued the theme of hydrogen bonding, covering the range from theory to applications. **Michael Zaworotko** had been scheduled to give the first lecture, but his place was ably taken by **Kari Rissanen**. Kari displayed a variety of cups and capsules in which conventional hydrogen bonding was important, but "new interactions" (anion…π, C-H…π, halogen bonding, C-H…anion) could also play a role. Resorcinarenes can offer 8 OH groups on the periphery, 4 R groups and 4 activated sites. Cavitands have a deeper bowl than resorcinarenes, but suitably substituted resorcinarenes can act as halogen-bonded analogues of deep-bowl cavitands. Next, **Pete Wood** showed us how the CSD can help us to understand the often vexing phenomenon of hydrate formation, which has a close relation to hydrogen bonding functionality. Anhydrate / hydrate systems occur for 38-75 % of small molecule drugs. Interconversion can lead to physicochemical instability, hygroscopicity of the anhydrate and variable uptake of water. A survey of 13,424 small (≤100 atoms) organic structures with no metals other than alkali showed that 6.6 % are hydrated. A subset comprising drugs exhibits a much larger proportion: 18.9 % are hydrated. Most drugs follow Lipinski's Rule of Fives, which could bias the sampling. There is no significant difference in molecular descriptors, but hydrate formers do have a lower log P. Functional groups do matter, and their nature is more important than their count. For instance, 14.5 % of triptans but only 2.4 % of sulphonamides exist as hydrates. Assessment of the hydrogen bonding environment of each unique H_2O shows that in ≈50 % of environments it is donating hydrogen bonds twice and accepting once. **Catherine Esterhuyzen** introduced a hydrogen bond acceptor that was new to many of us: gold. Gold is the most electronegative transition metal, and Au(I) can function as a Lewis acid. Its complexes are linear. Aurophilic attractive Au…Au interactions between two complexed Au(I) ions are well known, and auride ion (Au^-) is known to accept hydrogen bonds. Catherine presented calculations which showed that sufficiently electron-donating ligands can transform Au(I) into a Lewis base which is capable of accepting hydrogen bonds. **Filip Topić** directed our attention to applications through his work on synthetic routes involving hydrogen and halogen bonds to attain the challenging objective of making ternary cocrystals. Thioureas, phosphine oxides and various halogen bond donors were combined because combinations of two of them were known to yield binary cocrystals. Some ternary cocrystals were indeed obtained, based mainly around N-H…O hydrogen bonds between thiourea and phosphine oxides along with C-I…S halogen bonds between diiodo-tetrafluorobenzene and thiourea. Systematic exploration followed, whereby each possible binary mixture of the components was ground with the remaining component and the products formed were analysed. Subsequently, **Alankriti Bhajpai** returned our attention to crystalline hydrates. Desiraju proposed the principle that the proportion of hydrates should increase as hydrogen bond donors outnumber acceptors. But what should happen if there are no donors? This question was examined experimentally by hydrate screening of 11 organic compounds containing 5- or 6-membered heterocycles, of

which 6 compounds formed hydrates. An example is 1,2-bis(4-pyridyl)ethane, in which the crystal packing is influenced by two O-H…N hydrogen bonds bur also six π-π stacking interactions. Analysis of electrostatic potential and packing can also explain why no hydrates form with a particular compound.

The lecture programme ended with another brilliant Plenary Lecture by a Nobel laureate, this time **Jean-Marie Lehn**. For those of us who thought of chemistry primarily in terms of the making and breaking of covalent bonds, Jean-Marie opened up the exciting field of supramolecular chemistry. This type of chemistry is examining systems that can self-organize (spontaneously generate well-defined functional architectures from their components). He provided a wealth of examples, starting with molecular recognition. A cryptand plus a metal cation form a cryptate. Cages differing in size can optimally bind different alkali metal ions. Cylindrical molecular receptors exist for diammonium cations. Programmed self-organization can make use of electrostatic interactions and hydrogen bonding; the work presented here relied particularly on metal ion coordination. For instance, helicates can have double helices built from bipyridine and metal ions. Heterometallic grid architectures result from combining octahedral Zn(II) and tetrahedral Cu(I). Dynamics must be considered. For instance, the transoid form of 2,2'-bipyridine is 25 kJ mol^{-1} more stable than the cisoid form, but metal ion binding extends the range of possible conformations and could lead to construction of nanomechanical devices. If a double-helix former and a triple-helix former are mixed, they still form double and triple helices, not a muddle. Combining diversity and dynamics leads to adaptive chemistry. The non-covalent interactions are necessarily labile, but reversible covalent bonds can also be introduced, e.g. imine/carbonyl.

Carl Schwalbe

ECM30 in Basel started out for me on Monday morning with a fascinating lecture by Nobel laureate Ada Yonath talking about the structure and function of ribosomes. Other memorable talks that day were about mechanochemistry (T. Friščić), polymorphs (J. Bernstein) and layers in high Z' structures (C. Brock). After the talks I also had my poster session in the evening. The session was after a full day of talks and the posters quite crowded together, so attendance wasn't overwhelming. The day ended with refreshments and instrumental information provided by Bruker after which it was high time to find dinner and check out Basel.

Tuesday contained some nice talks on the simulation of dynamics in molecular crystals. The talks on polymorphism and phase transitions (**J. Nyman**) and on the computational dehydration of a hydrate (**A. Larsen**) were personally quite thought provoking. The light lunch provided by the conference was beefed up with refreshments and instrumental information by Rigaku Oxford Diffraction. This was followed by a session on the jungle that is crystal forms (of mostly pharmaceuticals). Thymine and orotic acid hydrates (**D. Braun**) and gabapentine (**M.T. Duarte**) were provided as intriguing cases from academia. There were also two different industry views (**C. Saal** and **U. Werthmann**) as well as help from the CSD to traverse the crystal form jungle (**N. Feeder**). Continuing with a related topic the keynote lecture of the afternoon was about organic crystal structure prediction (**M. Neumann**).

After the Tuesday poster session there was still more to come in the form of a Science Slam, where young scientists had 3 minutes to talk about their research in an entertaining and generally understandable manner. All the speakers did a very good job and received loads of applause made extra loud by small plastic hand clappers sponsored by Stoe. The Bertaut-Prize was given to **L. Reinhard**, and she gave a very good lecture on macromolecular crystallographic problems and solutions to end the evening.

Wednesday started out with a keynote by **S. Parsons** on phase transitions in molecular crystals, after which I joined the session on crystallography in art and cultural heritage, a field in which I have only recently become preoccupied. The afternoon session went back to my main interest in the form of hydrogen bonding, where we were linked to the previous session on the jungle of crystal forms by **P. Wood** discussing hydrates in view of the CSD. Additionally **F. Topić** presented some nice work on ternary cocrystals.

The conference dinner was in the evening and I took the chance to join a guided tour of the zoo beforehand. As we didn't get to choose our guide, I ended up learning more about birds instead of the perhaps more generally interesting big mammals. But I did spot some zebras and an orangutan in addition to exotic small birds and some pelicans before dinner, and even a bit of an elephant from the restaurant balcony.

The next morning started with a session on minerals, materials and polymorphs – a collective session which I had been asked to chair with **H. Hope**. It shaped up to be a nice session even though one of the speakers (luckily the last in the line-up) did not make it to the conference and the topic was quite broad. The talks by **M. Smets** on polymorphic transitions and **J. Gertenbach** on controlling porosity with temperature and pressure were personally interesting as they were close to my field. For the afternoon session I chose to hear more about the history of the ECA and crystallography and it was lucky I got there early as the lecture room was overflowing with interested listeners to hear about crystallography in Switzerland (**D. Schwarzenbach**), in the courtroom (**J. Bernstein**), about absolute structure (**H. Flack**), direct methods (**D. Viterbo**) and every crystallographer's favourite artist M.C. Escher (**H. Schenk**).

During afternoon coffee there was still time to loot the last of the freebies at the commercial exhibition. The exhibition ran all through the conference and was very nice as there were lots of competitions to take part in. I didn't win anything in the end, but competitions are a great way to open up a conversation with the exhibitors and learn about the newest advances in instrumentation, products and services. After coffee I attended the keynote by **M. Schmidt** on structure investigations of nanocrystalline and amorphous materials.

The closing plenary lecture was given by Nobel laureate **Jean-Marie Lehn**. He gave a fascinating talk looking to the future of supramolecular chemistry. Then it was time for the poster prizes and closing ceremony. Perhaps it was a statistical anomaly but the person sitting next to me won a poster prize, just like the four people sitting next to me at the closing of ECM in Warwick. I suggest you find me at the next ECM if you'd also like to win a poster prize.

Elisa Nauha
University of Lincoln

THE 30th meeting of the ECA was held in Basel, during a glorious period of hot weather when most of the inhabitants of the city seemed to be floating down the Rhine (an unusual but highly enjoyable experience by the way!). Over the five days we were treated to an extremely stimulating agenda of talks and posters, all presented to a very high standard and punctuated by plenty of time for discussions and networking. With difficulty, I've chosen four highlights to give you a taste of the week.

My first highlight – actually from before the start of the meeting proper – was the Crystallography in the Pharmaceutical Industry workshop. This satellite meeting brought together members of industry and academics with talks on topics as diverse as protein and small molecule crystallography, cryo-electron microscopy and HPC detectors. These talks were peppered with the speakers' personal experiences of crystallography in the pharmaceutical industry, an aspect I found particularly interesting. A reoccurring feature was the importance of cross-disciplines communication to enable fruitful collaborations and dissemination of knowledge. The day finished with a lively talk and discussion on careers in industry, focusing on how skills gained from crystallography are transferable to more diverse fields than we may imagine.

The second highlight was the opening plenary lecture by the Nobel Prize winner **Ada Yonath**. Her lively and accessible talk managed to cover the threat of global antibiotic resistance, the microbiome and the origin of life, just some of her work in the field of crystallography and ribosomes.

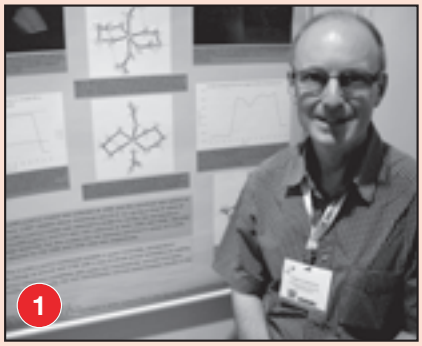
My third highlight was Professor **Makoto Fujita**'s keynote lecture, in which he eloquently and succinctly explained the work he and his group have done since first publishing their 'Crystalline Sponge' method in 2013. This technique enables the structural determination of non-crystalline compounds by SCXRD by encapsulating them inside a crystalline sponge framework. Whilst the technique had some initial setbacks, a huge range of previously unknown structures have now been elucidated; and, based on the work presented, we can look forward to a stream of new publications from his group alongside their many collaborators.

Last but not least, were the thoroughly enjoyable lectures in the General Microsymposia. Spread over a number of sessions, the talks focused on education, cultural heritage, art and the history of crystallography. Amongst others, we heard from crystallographer-artist **Anke Zürn** on Making Gold and an insight into her creative process, we were given a fun cross field perspective on symmetry by **Jean-Louis Hodeau**, and learnt about the use of crystallography in the examining the behaviour of pigments in heritage materials from **Koen Janssens**.

I would like to thank the BCA for providing a bursary for me to attend this conference. I certainly learnt a lot and came away inspired and energised to get to work on my own projects.

Lilian Hayes
University College London

Some presenters at ECM30



1. Mark Elsegood
2. Simon Parsons
3. Neil Feeder
4. Georgina Rosair
5. Pete Wood
6. Katharina Edkins
7. John Wallis
8. Laszlo Fabian
9. Sarah Gurung
10. Ralf Flaig

Annual Meeting of the German Crystallographic Society (DGK)

THIS meeting was held from 14-17 March at the institution where my father obtained his PhD many years ago, the University of Stuttgart. Sessions were held at the central campus, conveniently located near hotels, restaurants and tourist attractions, rather than at the out-of-town science campus. The organisers gave us an excellent opportunity to enjoy both culture and beer. They booked a block of tickets for us for a Tuesday evening performance of "Carmen" by the acclaimed Stuttgart Opera. I do not claim any expertise as a music critic or theatre critic, but most of my fellow crystallographers agreed with me that the singing was absolutely superb but the staging was most peculiar. The original plot, taut and psychologically well-judged, had been deconstructed, characters popping up where they were not expected. There was much stage business with floor lamps. While I also claim no expertise as a beer critic, the conference dinner in the restaurant of the Schönbuch brewery was a total success, the beer living up to its illustrious German reputation.

Professor **Susan Schorr**, Chair of the DGK, led an upbeat General Assembly, which had an excellent attendance not just because of German diligence but also because a free lunch was provided. Membership of the DGK stands at an impressive 1123, of which 861 are full members.

The first Plenary Lecture was literally a matter of life and death. **Karl-Peter Hopfner** told us about "Innate immune sensing and signalling of cytosolic DNA". This topic has been the subject of a review article by Hornung, Hartmann, Ablasser & Hopfner in *Nature Reviews Immunology,* **14**, 521-528 (2014). If viruses or bacteria introduce foreign DNA or RNA into a cell, or if the cell's own polynucleotides get damaged, there is no time to waste; the damage must be detected and dealt with immediately. For this reason the innate immune response has sensors which lead to signal transduction and a response. Neighbouring cells are warned by the production of interferon Nα/β, which binds to receptors on other cells, activating further interferon-regulated genes. Detection of cytosolic DNA, whether foreign or from damaged mitochondria, promotes the production of DNAse to degrade it. However, an imbalance in its control mechanisms can lead to autoimmune disease. The DNA damage recognition protein DisA is a dimer with the active sites facing each other; in 2008 electron density corresponding to no known amino acid was found in this interface region. It was identified as c-di-AMP, and this enzyme is now known to be a cyclic di-AMP synthase. Intracellular *Listeria* secretes c-di-AMP, which activates a host response via STING. STING is a direct sensor of c-di-GMP. STING structures appeared in 2012. As a last resort, 2′–5′-linked oligoadenylates activate the enzyme RNase L, which degrades both viral and host RNA, leading to complete shutdown of the infected cell. The cyclic GMP–AMP (cGAMP) synthase (cGAS) has a single active site but catalyses two distinct sequential reactions. It seems to require a nucleotide flip. An open question is why, given that 16-18 base pairs are enough to span a cGAS dimer, > 50 base pairs are required experimentally for its stimulation.

First speaker Prof Karl-Peter Hopfner with DGK President Prof Susan Schorr

Another lively Plenary Lecture was given by our own **Bill David** as part of the international celebration of 100 years of powder diffraction. It will not be summarised here because Bill also covered this topic at the BCA Spring Meeting.

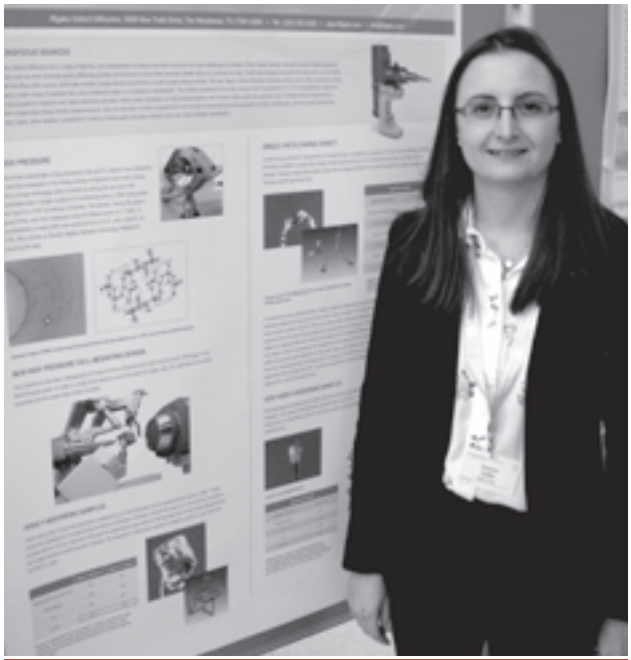
Another impressive Plenary Lecture was given by **Tomislav Friščić** on "Mechanochemistry and photo-mechanical effect". Tomislav started with a brief tour of his path through crystallography: doing small-molecule crystallography in Croatia, working with **Len McGillavray** in Iowa on solid-state dimer-forming photoreactions, working with **Bill Jones** in the UK on pharmaceutical co-crystals; and, since 2011, doing research in Canada on systems with even more components. He reminded us that solid-state reactions have been used since antiquity. In his work "On stones" **Theophrastus** described the preparation of liquid mercury by grinding cinnabar in a copper vessel with a little vinegar: $HgS_{(s)} + Cu_{(s)} \rightarrow Hg_{(l)} + Cu(S)_{(s)}$. The pigment white lead ($PbCO_3$) used to be prepared by exposing lead sheets to the vapour from rotting horse dung! In modern preparative methods involving the use of a mortar or a ball mill the material of the mortar or the balls is seldom documented but may be very important. Alternative theories about the mechanism of mechanochemistry have been proposed. Gilman (1996) attributed it to distortion of the HOMO and LUMO. In contrast, the Jones group proposed that surface layers move around, providing a new reaction environment. Now Tomislav aims to keep his laboratory solvent-free. Cyanoguanidine is a versatile reagent which can form 1:1 or 1:2 interactions. Templating and catalysis have been employed in MOF mechanosynthesis. A successful example is the ion- and liquid-assisted grinding together of ZnO, a cyclic diamine and 1,4-benzenedicarboxylic acid to form a MOF. The synthesis of ZIFs (zeolitic imidazolate frameworks) can be effected within minutes, monitored by PXRD.

In his talk "Charge density and disorder. New opportunities from invariom modelling" **Birger Dittrich** surprised us that these topics could coexist. He started by distinguishing static disorder, dynamic disorder and modulated structures. SHELX2015 has a wealth of tools for disordered structures in

the form of restraints to force the structure to become chemically reasonable. XD2006 offers few of these tools but provides better scattering factors. Multipoles are able to model disorder equally well to electron density. Birger presented four case studies. (1) A variable-temperature study of Me-AIB showed no disorder at 10 K or 30 K, but at 50 K disorder affected the whole ester group. Molecular dynamics simulation shows torsion angle jumps. (2) Re-analysis of DL-arginine monohydrate by invariom refinement against synchrotron data shows 2.7% disorder. Residual density analysis implemented by **J. Henn** and **K. Meindl** is a sensitive and incorruptible tool. (3) Whole-molecule disorder in Cefaclor has been sucesssfully modelled. (4) Glycyl-L-threonine has disorder of one water molecule.

Another lecture that taught me a lot of structural biology was by **Caroline Kisker** on "The good and bad of nucleoside excision repair". Nucleoside excision repair (NER) is the only human mechanism to repair UV-damaged DNA. Failure of this mechanism leads to the life-threatening disease xeroderma pigmentosum (XP); it may result from the malfunction of any gene in the group XPA to XPG, named in order of discovery. On the other hand, some cancer cells up-regulate their NER after treatment with cisplatin to get rid of the drug. XPD, also called ERCC2, is associated with a helicase which verifies damage to DNA. This helicase when isolated from *Thermophilum* is amenable to crystallographic study. Attempts to explain its mechanism showed the danger of over-interpretation of low-resolution data. The molecule has a wedge-shaped projection well placed to separate double-stranded DNA for verification. An obvious hole in the protein appeared to be a size gauge which would allow an intact strand to pass but would snag a bulky damage site. However, careful measurement of the hole size showed that it is too big to do this, and its function remains unknown. XPD has other roles, including cell cycle control. Mutants have been made to test which functions persist and which are abolished.

In the poster session my attention was particularly drawn to a poster by BCA Council member **Alexandra Griffin**. I have been accustomed to weighing up the relative merits of copper and molybdenum radiation for data collection, but Alex made a convincing case for considering silver as well. This is especially true for high-pressure crystallography, where the limited aperture of the cell restricts the range of Θ values of diffracted radiation that can be observed. The shorter wavelength of Ag radiation lets more reflections get through. The use of Ag radiation can facilitate charge density studies, and absorption is less of a problem with Ag than with Cu or Mo radiation.



Dr Alex Griffin with her poster

Dr Matthew Conroy giving his lecture

One of the final lectures was an informative and cautionary lecture by **Matthew Conroy** on "Protein Data Bank in Europe". Matthew reminded us that the worldwide PDB (wwPDB) consists of branches in the USA (PDB), Europe (PDBe) and Japan (PDBj). The assignment of data is geographical, with Africa and Europe contributing to PDBe. Regardless of geography, the data end up in a common archive. Too often "small molecules" in the PDB have dreadful geometry [J. Liebeschuetz, J. Hennemann, T. Olsson & C. R. Groom, *J Comput Aided Mol Des* (2012) 26: 169. doi:10.1007/s10822-011-9538-6]. Matthew cited a critique [E. Pozharski, C. X. Weichenberger & B. Rupp, *Acta Cryst.* (2013). D**69**: 150. doi:10.1107/S0907444912044423] of a structure where a crystal was soaked with a ligand but there was no evidence that the modelled ligand had actually bound! The wwPDB provides access to validation servers that structural biologists can use to validate their models.

Carl Schwalbe

Stanley C. Nyburg
(1924-2016)

Professor Stanley C. Nyburg was born in London in 1924. After a childhood that included being a wartime evacuee, he obtained an honours degree in chemistry, with a physics subsidiary, having studied part-time at Birkbeck College, London. After a year at King's College, London, he began work as a crystallographic trainee at the British Rubber Producers' Research Association (BRPRA), an Institution of London University, where he first met George Jeffrey ('Jeff'), who was later to become his PhD supervisor following a move to the University of Leeds. There he solved the crystal structure of an organic compound by photographic film methods, a considerable achievement at the time, before taking up an appointment as assistant lecturer at the new University College of North Staffordshire at Keele in 1949. At Keele, together with colleagues he built an X-ray generator, determined Bragg intensities photographically and determined a number of crystal structures including a natural product that had resisted structural characterization despite over 40 years of intense chemical study.

In 1958 he rejoined George Jeffrey, then at the University of Pittsburgh, as a Fulbright Fellow, and began investigations into how crystalline Cl_2 came to have its extraordinary herringbone structure. This led, some years later, to a CSD study of non-bonded distances between identical atomic elements, showing for the first time, that for the halogens especially, the effective van der Waals shapes are not truly spherical but flattened.

In 1963 Stan took up the post of full professor at the University of Toronto in the new Department of Chemistry, where start-up funds enabled the purchase of an early automated diffractometer, in this case a four-circle Picker machine. This proved a good choice, the machine being in subsequent operation for more than 40 years, 23 of which were at Toronto where the diffractometer was employed in provision of a crystal structure determination service. A highlight of that period was Stan's determination in 1965 of the structure of a ruthenium compound, which first established the capability of dintrogen as a ligand. Further key contributions included the crystal structures of a number of long-chain *n*-alkanes.

In 1987 Stan returned to King's College, London, as an honorary senior fellow, bringing with him the Picker diffractometer, which Kings purchased for a few thousand dollars. As Stan later recounted, "Its delicate goniometric parts were covered in a slow-setting sheath of polystyrene by someone who had done similar work for Ford automobile engines. It was shipped (all 0.75 tons) over the Atlantic in a Russian freighter to London, UK. The Picker was newly fitted to a PC, an IBM 286, and Eric Gabe's Fortran program for data collection was rewritten in Gbasic." The Picker behaved excellently and was used to determine a large number of crystal structures for research groups at Kings College. After the closure of the Department of Chemistry at Kings College in 2006, Prof. Nyburg took up an honorary senior fellow appointment at University College, London and was able to continue his studies of *n*-alkanes.

King's College holds an archive of Prof. Nyburg's papers, which can be accessed by contacting the archivist at http://www.kcl.ac.uk/library/archivespec/archives/access.aspx.

Lee Brammer, President of the British Crystallographic Association

Michael James, Canadian Representative of the American Crystallographic Association

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.

12-16 December 2016
New Trends in Magnetic Structure Determination, Grenoble, France.
https://indico.ill.fr/indico/event/53/

13-16 December 2016
Structural Biology meets Biophysics, Obernai, France.
http://sfb-gtbio2016.u-strasbg.fr/index.php

13-20 December 2016
DLS-CCP4 Data Collection and Structure Solution Workshop, Harwell.
http://www.ccp4.ac.uk/schools/DLS-2016/

14-16 December 2016
From Matter to Materials and Life. A science workshop, Hamburg, Germany.
https://indico.desy.de/conferenceDisplay.py?confId=15714

19 December 2016
Biological Structures Group Winter Meeting 2016, London.
http://bsg.crystallography.org.uk/wint16.html

3-6 January 2017
ASU Electron Microscopy Winter School, Tempe, AZ, USA.
https://le-csss.asu.edu/winterschool

6-7 January 2017
Cryo-EM Workshop of the ASU TEM Winter School, Tempe, AZ, USA.
https://le-csss.asu.edu/winterschool

9 January 2017
Single Particle Workshop. In conjunction with the 4th Annual BioXFEL STC International Conference, Las Vegas, NV, USA.
https://www.bioxfel.org/events/details/1125

9-11 January 2017
CCP4 Study Weekend, Nottingham.
https://eventbooking.stfc.ac.uk/news-events/ccp4-study-weekend-2017-344

9-13 January 2017
Theory Winter School. Modeling of Correlated Electron Materials, Tallahassee, FL, USA.
https://nationalmaglab.org/news-events/events/for-scientists/winter-theory-school

10-12 January 2017
BioXFEL STC 4th Annual International Conference, Las Vegas, NV, USA.
https://www.bioxfel.org/events/details/1093

17-18 January 2017
LiXS 2017: Liquid X-ray Spectroscopy, Gif-sur-Yvette, France.
http://www.synchrotron-soleil.fr/portal/page/portal/Soleil/ToutesActualites/Workshops/2017/LiXS2017/Accueil

18-20 January 2017
Electronic Materials and Applications 2017, Orlando, FL, USA.
http://ceramics.org/EMA2017

19-20 January 2017
12th Soleil Users' Meeting, Gif-sur-Yvette, France.
http://www.synchrotron-soleil.fr/

25-27 January 2017
Joint DESY Photon Science and European XFEL Users' Meeting: Research with Synchrotron Radiation and FELs, Hamburg, Germany.
http://photon-science.desy.de/users_area/users'_meeting/index_eng.html

26-27 January 2017
RSC Chemical Nanosciences and Nanotechnology Network Meeting, Keele.
http://www.rsc.org/events/detail/23918/rsc-chemical-nanosciences-and-nanotechnology-network-meeting

5-9 February 2017
42nd Lorne Conference on Protein Structure and Function, Lorne, VIC, Australia.
http://www.lorneproteins.org/

6-8 February 2017
ESRF User Meeting 2017, Grenoble, France.
http://www.esrf.eu/UM2017

11-15 February 2017
61st Annual Meeting of the Biophysical Society (with new Cryo-EM Subgroup meeting), New Orleans, LA, USA.
https://www.biophysics.org/2017meeting/Home/tabid/6672/Default.aspx

12-16 February 2017
AMN-8 8th International Conference on Advanced Materials and Nanotechnology, Queenstown, New Zealand.
http://confer.co.nz/amn8/

19-22 February 2017
5th Banff Meeting on Structural Dynamics, Banff, Alberta, Canada.
https://banff2017.desy.de/

27 February – 30 March 2017
HERCULES European School, Grenoble, France.
http://hercules-school.eu/

2-7 March 2017
ICCOSS XXIII, 23rd International Conference on the Chemistry of the Organic Solid State, Stellenbosch, South Africa.
http://iccoss2017.co.za/

6-8 March 2017
Towards novel therapies: Emerging insights from structural and molecular biology, Groningen, Netherlands.
http://events.embo.org/17-structural-biol/

13-17 March 2017
APS March Meeting 2017, New Orleans, LA, USA.
https://www.aps.org/meetings/meeting.cfm?name=MAR17

16-18 March 2017
3rd Annual World Congress of Smart Materials (WCSM-2017), Bangkok, Thailand.
http://www.bitcongress.com/wcsm2017/ScientificProgramme_sm.asp

19-22 March 2017
XXIII West Coast Protein Crystallography Workshop, Pacific Grove, CA, USA.
http://www.biochem.utah.edu/hill/wcpcw.html

21-23 March 2017
2017 International Conference on Frontiers of Characterization and Metrology for Nanoelectronics(FCMN), Monterey, CA, USA.
http://www2.avs.org/conferences/FCMN/

22-24 March 2017
5th Annual Conference of AnalytiX, Fukuoka, Japan.
http://www.bitcongress.com/Analytix2017/

25 March – 2 April 2017
16th BCA/CCG Intensive Teaching School in X-Ray Structure Analysis, Durham.
http://community.dur.ac.uk/durham.x-ray-school/staff.htm

26-31 March 2017
International Workshop on Photoionization (IWP) & Resonant Inelastic X-ray Scattering (RIXS), Aussois, France.
http://www.synchrotron-soleil.fr/Workshops/2017/IWP-RIXS2017

29 March – 11 April 2017
Expression, Purification & Analysis of Proteins and Protein Complexes, Cold Spring Harbor Laboratory, NY, USA.
https://meetings.cshl.edu/courses.aspx?course=C-PPC&year=17

29 March – 11 April 2017
Quantitative Imaging: From Cells to Molecules, Cold Spring Harbor Laboratory, NY, USA.
https://meetings.cshl.edu/courses.aspx?course=C-QICM&year=17

10-13 April 2017
BCA Spring Meeting, Lancaster.
http://www.crystallography.org.uk/bca-spring-meeting-2017-programme-committee/

17-21 April 2017
MRS Spring Meeting & Exhibit, Phoenix, AZ, USA.
http://www.mrs.org/spring2017/

18-21 April 2017
International Conference on Laser Energy Science / Laser and Accelerator Neutron Sources and Applications, Yokohama, Japan.
http://lansa.opicon.jp/

22-26 April 2017
Hot topics in contemporary crystallography (HTCC), Poreč, Croatia.
http://www.htcc2017.org/

24-28 April 2017
INTERMAG Europe 2017. IEEE International Magnetics Conference, Dublin, Ireland.
http://intermag2017.com/

14-19 May 2017
Protein quality control. Success and Failure in Health and Disease. Sant Feliu de Guixols, Spain.
http://events.embo.org/17-quality-control/

21-23 May 2017
EMBO/EMBL Symposium: Molecular and Cell Biology of Membranes, Heidelberg, Germany.
http://www.embo-embl-symposia.org/symposia/2017/EES17-03/index.html

22-26 May 2017
E-MRS Spring Meeting and Exhibit, Strasbourg, France.
http://www.european-mrs.com/meetings/2017-spring-meeting

25-26 May 2017
Instruct Biennial Structural Biology Meeting (IBSBM2017), Brno, Czech Republic.
https://www.structuralbiology.eu/update/biennial2017

26-30 May 2017
Annual Meeting of the American Crystallographic Association, New Orleans, LA, USA.
http://www.amercrystalassn.org/content/pages/main-annual-meetings

2-11 June 2017
International School of Crystallography 50th Course: Integrative Structural Biology, Erice (Sicily), Italy.
https://crystalerice.org/2017/

5-7 June 2017
canSAS: Small Angle Scattering Workshop, San Francisco, CA, USA.
https://sites.google.com/a/lbl.gov/cansas/home

11-22 June 2017
The Zurich School of Crystallography 2017: Bring Your Own Crystals, Zurich, Switzerland.
http://www.chem.uzh.ch/linden/zsc/

12-21 June 2017
Joint FEBS-EMBO Advanced Lecture Course: Molecular Architecture, Dynamics and Function of Biomembranes, Cargèse, Corsica, France.
http://web.science.uu.nl/cargese2017/

19-23 June 2017
Mineral Fibres: Crystal Chemistry, Chemical-Physical Properties, Biological Interaction and Toxicity, Modena, Italy.
http://emu2017.unimore.it/wp-content/uploads/2016/03/EMU2017_flyer.pdf

3-6 July 2017
Microscience Microscopy Congress 2017, Manchester.
http://www.mmc-series.org.uk/

9-13 July 2017
International Conference on Neutron Scattering 2017, Daejon, Republic of Korea.
http://www.icns2017.org/

10-13 July 2017
13th International Conference on Materials Chemistry (MC13), Liverpool.
http://www.rsc.org/events/detail/21273/13th-international-conference-on-materials-chemistry-mc13

16-20 July 2017
19th IUPAB Congress and 11th EBSA Congress, Edinburgh.
http://www.iupab2017.org/home

24-28 July 2017
9th International Conference on Borate Glasses, Crystals and Melts and 2nd International Conference on Phosphate Glasses, Oxford.
http://www.borate-phosphate.sgt.org/

30 July – 4 August 2017
21st American Conference on Crystal Growth and Epitaxy (ACCGE-21) and 18th US Workshop on Organometallic Vapor Phase Epitaxy (OMVPE-18), Santa Fe, NM, USA.
http://www.crystalgrowth.org/Santa-Fe.html

14-15 August 2017
International Workshop on Improving Data Quality in XAFS Spectroscopy, Diamond Light Source.
http://www.diamond.ac.uk/Home/Events/2017/Q2XAFS2017.html

18-21 August 2017
Pharmaceutical Powder X-ray Diffraction Symposium, Hyderabad, India.
http://www.icdd.com/ppxrd

21-28 August 2017
24th Congress of the International Union of Crystallography, Hyderabad, India.
http://www.iucr2017.org

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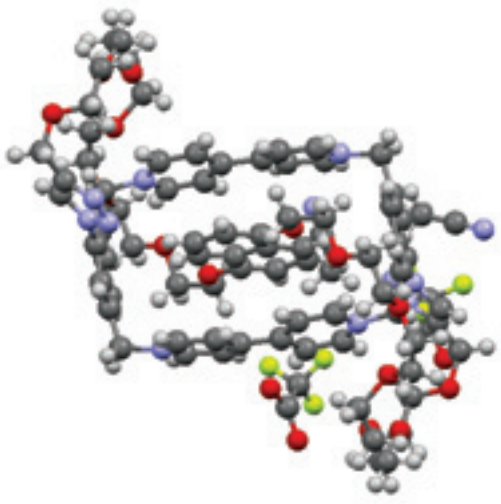

A rotaxane published by a group of authors including Nobel Prize winners Sauvage and Stoddart. This structure was a CCDC Friday Feature on Twitter.

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30 years

of designing, understanding and improving low temperature devices for crystallography

60 countries

in which our low temperature devices are used

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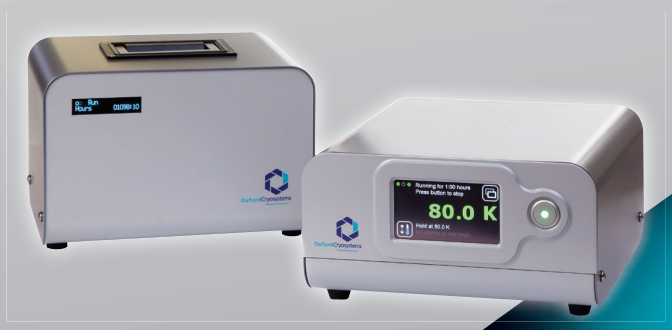

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