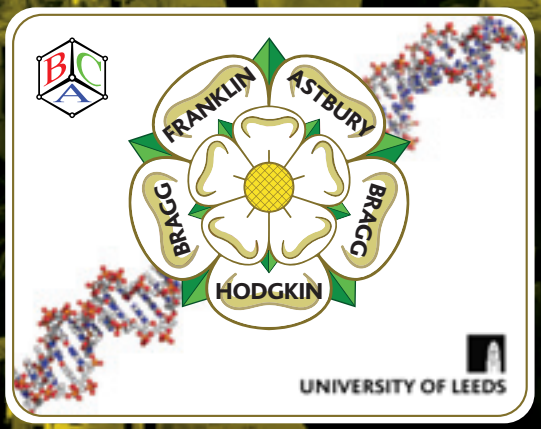
Crystallography News

British Crystallographic Association

Issue No. 150 September 2019
ISSI 1467-2790



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Spring Meeting Preview p6
ACA Meeting Reports p8
The IYPT Crystals Project p11
The CSD Reaches 1 Million Entries! p12
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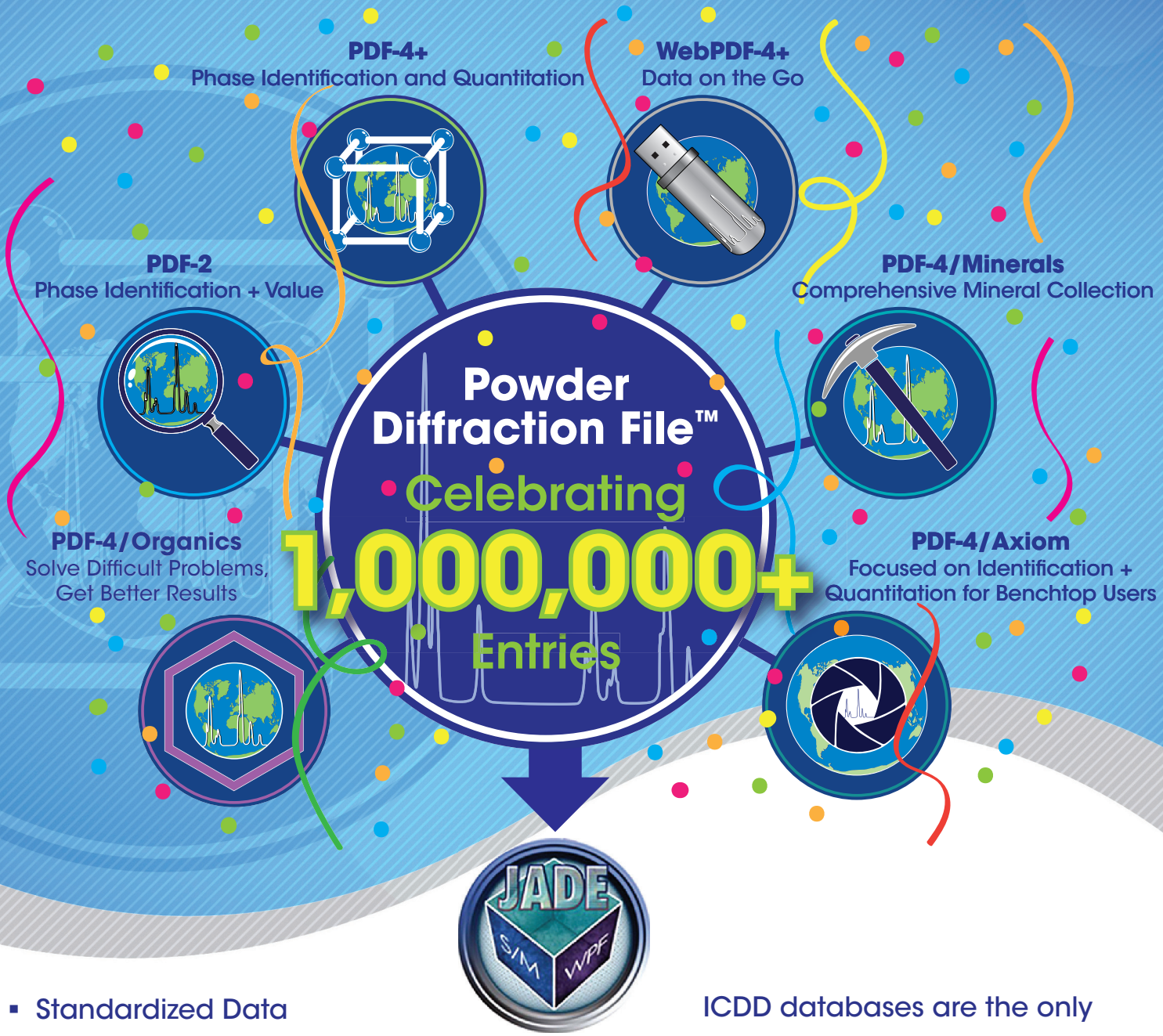

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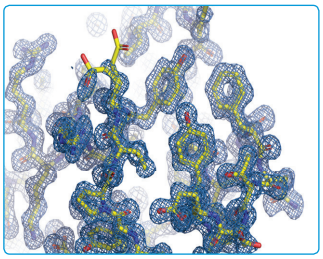

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By Hook or by Crook – Structural Solutions from Challenging Crystals

BCA Industrial and Chemical Groups

Joint Autumn Meeting

20th November 2019, GSK, Stevenage, Herts, SG1 2NY.

BCAIG

BCA Industrial Group

Please come along to our joint autumn meeting. Sessions will cover non-traditional structure solutions, industrial applications for powder diffraction and the CCG/CCDC 2019 prize lecture.

Confirmed speakers include:

- Dr Lukáš Palatinus (The Czech Academy of Sciences)
- Prof Alastair Florence (Strathclyde, CMAC)
- Dr Mathilde Reinle-Schmitt (Excelsus SLS)
- Dr Dominik Daisenberger (Diamond, I15)

Registration will open on 1st September, for full details see our website www.industrial.crystallography.org.uk

THE WINTER CRYSTALLOGRAPHY MEETING

of the Physical Crystallography Group (Structural Condensed Matter Physics Group)
ISIS Crystallography User Group
and Diamond Crystallography Group

will be held on

Monday 4 and Tuesday 5 November 2019
at **Milton Hill House, Steventon, Oxfordshire, UK**

Programme will include presentation of the 2019 ***Malvern Panalytical*** *Thesis Prize winner*

Thanks to generous sponsorship from **ISIS Neutron and Muon Source** and the **Institute of Physics**, there is no registration fee. Registration will open in September 2019.
For further details please see our website **www.pcg-scmp.org**.

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This month's cover:

Celebrating CSD 1 million (photos by Suzanna Ward) and the Leeds 2020 Spring Meeting logo

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CRYSTALLOGRAPHY NEWS is published quarterly (March, June, September and December) by the British Crystallographic Association, and printed by North Wolds, York. 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 December 2019 issue are sent to the Editor to arrive before 25 October 2019.

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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.

Printed by North Wolds Printers
83 Halifax Way, Pocklington Industrial Estate, Pocklington, York, YO42 1NR
Tel: 01759 303944
Web: www.northwolds.co.uk

From the President

THIS issue does not have the usual letter from Carl Schwalbe as Editor. BCA members will be greatly saddened to learn that Carl passed away on 1st August, following a short illness. Carl was a major, and much loved, figure in the BCA, combining editing *Crystallography News* for over 10 years with writing major articles on eminent crystallographers and, of course, his research in medicinal chemistry. He will be sorely missed in our community. Simon Coles kindly volunteered to stand in as editor for this issue, and I would like to extend my thanks to him for his efforts. It is a complex task, which we can easily forget given the apparent ease and efficiency with which Carl handled it. Simon's editorial column looks back at Carl's contribution as editor over the years.

I was waiting with baited breath on the 15th July for the announcement from the Bank of England on which scientist would feature on the new £50 note. Readers will remember that there were two crystallographers on the shortlist, **Dorothy Hodgkin** and **Rosalind Franklin**. In the event, it was **Alan Turing**, a very worthy choice, but I could not hide a slight feeling of disappointment that it was not a crystallographer in the end.

As members will know, 2019 is the International Year of the Periodic Table, marking the 150th anniversary of the **Mendeleev** periodic table. Perhaps less well known is that July 2019 is the 100th anniversary of the birth of **Primo Levi**, chemist and author of the wonderful book entitled simply The *Periodic Table*. In 2006, the Royal Institution named it as the best science book ever written, a view I find it hard to argue with. I would urge every chemist to read it, in fact anyone with any interest in science and human nature. He was a great author, but continued to work as a chemist for his entire career. A nice article on Levi appears in the July 2019 issue of *Chemistry World*.

Readers of my two previous letters might have concluded that I am interested in chirality. While in the 6th form at school, or school year 13 as it is now known, I read a little book called *The Ambidextrous Universe* by **Martin Gardner**, who used to write mathematics puzzles in *Scientific American*. He discusses Parity, the equivalence, or otherwise, of things related by inversion of all three coordinates in space, i.e. the mirror world. He coined the term the *Ozma Problem* to describe the difficulty we would have in communicating our definition of left and right to an intelligent civilization on a distant planet using radio waves. In fact, the only physics experiment (that we know of) where Parity is broken is measurement of the asymmetry of β- and γ-emission from Cobalt 60 nuclei relative to their nuclear spin. The crucial experiment was carried out by **Chien-Shiung Wu** in 1956. She did not receive the Nobel Prize for this work, and it went instead to **Lee** and **Yang**, the theoretical physicists who originated the idea. The weak nuclear force appears to be the only way that mirror-related worlds would differ.

As many crystallographers will know, the crucial experiment that revealed the importance of the chirality of molecules was done by **Louis Pasteur**. Winemakers at the time wanted to know why wine went off when exposed to air, and contracted Pasteur to find out. Pasteur noticed that crystals of tartrate were often found in wine sediment. When studied under a microscope it was clear their crystal habit was asymmetric, i.e. had a hand, and all the crystals from wine had the same hand. He also noted that chemically synthesized tartrate crystals are a mixture of left and right-handed forms. A solution of this mixture would not rotate the plane of polarization of light, while a solution of crystals taken from wine did produce a rotation. He separated individual synthetic crystals of the two forms under a microscope, and showed that solutions of each would rotate the plane of polarized light, but in opposite directions depending on the hand. His conclusion was that the underlying molecules must also have a hand, and the ones from a biological source were only of one kind. He presented this work to the Académie des Sciences in Paris in 1848. There is a wonderful quote from him that translates as *"There are wonders hidden in crystallisation, and, through it, the inmost constitution of substances will one day be revealed"*. Crystallography rules OK!

Pasteur's apartment and laboratory are preserved as a museum in the original building at the Institut Pasteur in Paris. In the lab are little piles of his tartrate crystals, along with other wonderful artefacts. His paper was probably read by Lewis Carroll before writing *Through the Looking Glass*, and *What Alice Found There* (1871) where the book is woven around ideas of equivalence of, or difference between, left and right. In an early scene, Alice looks in a mirror at her reflection, and that of her cat, and says *"How would you like to live in Looking-Glass House, Kitty? I wonder if they'd give you milk in there? Perhaps Looking-Glass milk isn't good to drink?"*. The answer is that it is probably good for a looking-glass cat but not very nourishing for a normal one. There are numerous other references to mirror symmetry, including Tweedledum and Tweedledee (are they twins or mirror images?) and the white knight trying to put his right foot into his left shoe. Arguments continue about Parity at the molecular scale, and a paper was published by Belo *et al* in the *IUCr Journal* in 2017, claiming a lack of equivalence between crystalline D- and L-Alanine. This was contested by Bürgi and Macchi, in *IUCr J* in 2018.

On a further sad note, I am sorry to report the death of **Michael Rossmann**, a true giant in macromolecular crystallography. Michael was not BCA member, but will be well known to many of us. He was responsible for major advances in phasing and structure determination, most notably in molecular replacement and symmetry averaging. Amongst achievements too numerous to mention are the crystal structure of the common cold virus, the Rossmann fold in proteins, the EM structure of Zika virus, and the Ewald and Aminoff Prizes.

Planning for the 2020 Spring Meeting in Leeds is well advanced, and an outline programme appears elsewhere in this issue. Members should note that nominations for elections to BCA Council for Treasurer and Ordinary Member are due by 30th September. **Elizabeth Shotton** and **Hazel Sparkes** currently hold these positions, and are eligible for re-election.

Simon Phillips

BCA Council 2019

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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

IT is with some considerable sadness that I find myself guest editing this issue of *Crystallography News* at short notice. By the time you read this column you will likely be aware that our regular editor, Carl Schwalbe, found he had a very serious illness in early July and had to stand down from all work-related activities with immediate effect. On 1st August Carl passed away and our/my feelings go out to his wife Joan and their two sons who were with him at the end.

On a shelf in my office I have every edition of *Crystallography News* going back to the late 80's – the shelf is beginning to bow somewhat! What is so striking to me is that the proportion that Carl has been responsible for is so significant – his first edition of *Crystallography News* was June 2008, which occupies a third of this shelf. Only now do I truly appreciate the amount of sheer effort that has gone into producing this quarterly magazine, which as a professional society newsletter is exemplary and in itself more than justifies the membership fee! Carls incredible enthusiasm for *Crystallography News* was infectious, as all those who have been approached by him to write a piece will testify – his kind and supportive approach to being Editor meant everyone delivered!

So, to reflect both on the position I find myself in and also showcase Carl's work over the last decade, I thought I would flick though some back issues of *Crystallography News*. Perhaps I should have guessed that this idle 'task' would have taken more time than I expected – I got totally sucked in with reminiscing and it took up way more time than I could afford! However, I thought I would jog a memory or two out there by noting some of my favourite top 10 pieces over this time.

1) I will start with a bit of a cheat, as this was a theme spread over several issues, – I recall finding the insights/updates to our central facilities (2008-2010) very useful summaries that particularly highlighted crystallographic activities at these very large centres.
2) An introductory tutorial to dual-space phasing (June 2009) attracted my attention as I had been talking about it with laser science colleagues – one of the authors, Pierre Thibault has subsequently become a colleague in our Physics department.
3) There was a great piece (Sept 2012) on the Two Braggs – clearly a warm up for the celebrations of crystallography in the following two years.
4) The 'how we X-rayed Mars' feature (March 2013) is a little dog-eared, as I have used it a number of times to illustrate to school children just how useful/cool crystallography is!
5) *Crystallography News*, particularly under Carl, has always been a great way of finding out what has been going on at conferences around the world – the piece de resistance of Meeting Reports quite simply has to be the one on ECM28, which we hosted in Warwick (Dec 2013).
6) The International Year of Crystallography was a real turning point for Education and Outreach and so the March 2014 issue that describes a range of activities has to go down as a great.
7) I am an out-and-out data nerd, so feel that the 50-year celebration of the CSD (Sept 2015) really illustrates how crystallography leads the way here.
8) 'UK crystallographers collaborate with Africa' (Sept 2016) kicked off a number of subsequent features about crystallographic activities on this continent, which is a topic very dear to my heart.
9) Carl received Honorary BCA membership last year (June 2018).
10) The publication of the BCA Equality, Diversity and Inclusion policy is a really important and leading stance for our organisation to take (June 2018).

Many of these articles would not have come to pass if it weren't for Carl's kind natured tenacity – and in fact he actually authored some, can you identify which ones?

And so on to the here and now…

My Twitter feed was lighting up in early June due to the arrival of the 1,000,000th entry into the CSD. I can only imagine that there was quite a lot of pacing up and down, like expectant parents, in the corridors at CCDC during this time! This is such a significant milestone for our community, as it not only illustrates the massive contributions from a worldwide community and the > 50 year effort to collate these, but to me it signifies the advent of data really driving the science we do and in fact being a science in itself. For this reason, I consider this issue of *Crystallography News* to be a celebration of this community achievement. As an Honorary Senior Research Fellow at CCDC, I know for sure that you will approve of this Carl!

I would also like to note that Puzzle Corner has been put together by Carl's predecessor – **Bob Gould**. I am delighted that Bob could find time to do this and it's wonderful that this issue could be marked with a contribution from someone that has already devoted so much to the BCA and to *Crystallography News* – welcome back for this issue Bob!

As I write the summer conference season is upon us – I made a vow back at Christmas that I wasn't going to travel so much this summer, but with so many interesting meetings, I completely failed to keep to it! We have a number of meeting and school reports in this issue from the Easter season, along with a preview of our own Spring Meeting, which will be held in Leeds next year.

I'd also like to draw your attention to the IYPT Crystals article. This is a project that was conceived by **Claire Murray** and CCDC have picked it up and really run with it. The basic idea is to engage members of the community to write up an entry for an element, partly based on a notable crystal structure that contains that element. Having done a couple myself I can definitely say that it was fun to do and I encourage you to get involved and thereby be added to our list of contributors. We are hoping that a small grant from the RSC can help make sure this becomes a resource that is used for education and outreach.

I have been struck by the warmth of feeling for Carl from the community. This issue has been put together really quite rapidly and from very little background or starting point, however within hours of me sending pleading messages out, colleagues were pulling out all the stops to help and to produce materials. I'd like to thank those involved for pulling together at such short notice.

This edition of *Crystallography News* is for you Carl – Thanks a Million!

Simon Coles

BCA Corporate Membership

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.
- 10% discount on exhibition stands at the annual BCA Spring meeting.
- Free insert in the annual Spring Meeting delegate pack.
- Two free non-residential registrations to the annual Spring Meeting.
- Ten complimentary copies of the quarterly Crystallography News.
- Corporate Members will be listed in every Crystallography News and on the BCA website with clickable links to your organisation's website.

From 2019, corporate membership will be **£800.00** for one year.

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- A broad range of meetings organised by the BCA and its subject groups
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- A copy of Crystallography News every quarter
- Optional E-mail notifications of news items and meeting information
- Influence on the development of crystallography and the BCA

For current rates, and to join, please see **www.crystallography.org.uk/membership/**

Puzzle Corner

AFTER managing to stay away from *Crystallography News* for over a decade, **Bob Gould** was persuaded back to set a Puzzle Corner. Good luck, its fiendishly technical…!

It's sometimes convenient to use an alternative setting of a space group (for instance to compare a structure in $P222_1$ with another in $P2_1$ when the c-axis of one structure corresponds to the b-axis of the other). But it's also easy to make a mistake. Which of the following correspond to possible transformations and which do not?

	Standard	Transformed?
1.	Pbca	Pcab
2.	Pbca	Pcba
3.	$Pa\bar{3}$	$Pc\bar{3}7$
4.	$Pa\bar{3}$	$Pb\bar{3}$
5.	C2/c	A2/a
6.	P23	P32
7.	$P\bar{4}2c$	$P\bar{4}c2$
8.	Cmm2	Amm2

Answers to June Puzzle Corner

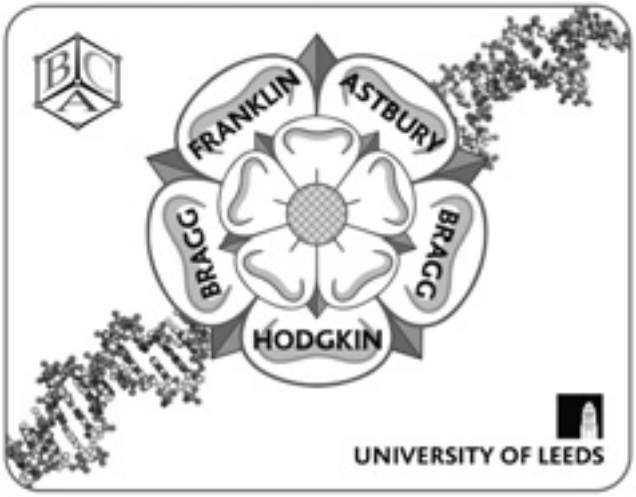
CARL set the following puzzle for you all, but we don't have his answers! Here's my thoughts on some responses, but if you know of alternatives or would like to point out errors or additions please email me (s.j.coles@soton.ac.uk) and we will publish a crowd-sourced set of answers in the next issue!

In this Year of the Periodic Table our Programme Committee succeeded in constructing our society's initials out of element symbols. With the order changed and a number added, CaB_6 is a fascinating material with high electrical conductivity, hardness and melting point. It is a black, lustrous, chemically inert powder with a low density. It exhibits unusual high-temperature ferromagnetism. Its structure is cubic.

Can you make the following sets of initials of some of our sister crystallographic societies out of element symbols? Identify the country as well.

ACA	???		**United States of America**
AFC	CaF_2	[known material]	**France**
CSCA	CaCs		**Czech Republic and Slovakia**
DGK	GdK		**Germany**
ICA	CaI_2	[known material]	**India**
ICRA	$CaIr_2/Ca_5Ir$	[known materials]	**Ireland**
NVK	KVN_2	[known Heusler compound]	**Netherlands**
PTK	PtK	[known alloy]	**Poland**
SGK	SgK		**Switzerland**
SMCr	SmCr	[known 'melt' phase]	**Mexico**

BCA Spring Meeting 2020
6th – 9th April 2020, University of Leeds



PLANNING is well underway for the 2020 BCA spring meeting to be held in Leeds, so please put the dates in your diaries! Details and titles for sessions are given below to give you time to think ahead to the abstract deadlines in January 2020.

Monday 5th April – Tuesday 6th April:
YCG meeting

The YCG satellite meeting is an opportunity for all early career researchers in the field of crystallography to present their work in a supportive and friendly environment, which will be run by fellow early career scientists.

YCG Opening Plenary –
Dr **Ehmke Pohl** (Durham)
(Chairs: Natalie Tatum/Tom Roseveare)

YCG Research Sessions
Contributed talks from the YCG community.
(Session 1 Chairs: Natalie Tatum/Tom Roseveare)
(Session 2 Chairs: Elliot Carrington/Charlie McMonagle)
(Session 3 Chairs: Aly Abedeldaim/Tom Roseveare)

Parkin lecture – recipient tbc
(Chair: Charlie McMonagle)

YCG/IG Session – title tbc
(Chairs: Natalie Johnson/Rachel Wilkinson)

YCG Closing Plenary –
Dr **Cheryl Doherty** (GSK)
(Chairs: Elliot Carrington/Charlie McMonagle)

Londsdale Lecture – recipient tbc
(Chair: Aly Abedeldaim)

Tuesday 6th April – Thursday 8th April:
Main Meeting

BSG Plenary Lecture: Rosalind Franklin Centenary Lecture
Professor **Gabriel Waksman** (UCL/Birkbeck)
Mechanism of effector targeting by the Legionella type IV secretion system
(Chair: tbc)

PCG: Biominerals & biomaterials
(Chair: Julia Parker, Diamond)

CCG: Advances in software for crystallography
(Chair: tbc)

BSG: Structure-based drug design
(Chair: Jane Endicott, Newcastle)

PCG: Entropy & structure
(Chair: Anthony Phillips, Queen Mary University London)

CCG: Electron crystallography
(Chair: tbc)

BSG: Time resolved crystallography
(Chair: Briony Yorke, Leeds)

PCG Plenary:
Professor **Vaclav Petricek** (The Czech Academy of Sciences)
The role of crystal structure analysis in investigation of crystals with important physical properties
(Chair: Anthony Phillips, Queen Mary University London)

Wednesday 9th April 2019

IG plenary:
Dr **Marcus Neumann** (Avant Garde Materials Simulation)
Detecting and avoiding disappearing polymorph cases by crystal structure prediction
(Chair: tbc)

IG/BACG: Crystal growth/pitfalls and challenges
(Chair: tbc)

PCG: <3D
(Chair: tbc)

BSG: Enzymes
(Chair: Wyatt Yue, Oxford)

More sessions to be announced

IG/CCG: Control & prediction of crystals
(Chair tbc)

PCG: >3D
(Chair: **Phil Lightfoot**, St Andrews)

BSG: Computational biophysics
(Chair: **Matteo Degiacomi**, Durham)

Bragg Lecture:
To be announced – Lecturers are chosen by the Bragg Lecture Fund Committee once every three years and the lecture is one of the highlights of the British Crystallographic Association Spring Meeting programme.

BCA AGM and conference dinner followed by ceilidh

Thursday 9th April 2019

CCG Plenary:
Dr **Franziska Emmerling** (Federal Institute for Materials Research and Testing (BAM))
(Chair: tbc)

CCG: Chemistry at extreme conditions
(Chair: **Hamish Yeung**, Oxford)

CCG/PCG: Structure solution from powders
(Chair: **Karen Johnston**, Durham)

BSG: Membrane proteins
(Chair: **Bonnie Wallace**, Birkbeck)

PCG Phase transitions
(Chair: **Lewis Owen**, Cambridge)

CCG: Hot & cold structures
(Chair: tbc)

BSG: Protein-protein interactions
(Chair: **Richard Bayliss**, Leeds)

ACA Conference Reports
July 20-24, 2019

THIS was the 69th Annual Meeting of the American Crystallographic Association and whose overall heading was "Convergent Structural Science". Some 550 registrants and 450 presenting authors gathered at the Northern Kentucky Conference Centre linked by a short walkway to the Marriott Hotel. I was also here at the 2003 ACA Conference and my excellent memories of that meeting were again amply rewarded by a thoroughly engaging set of presentations. The venue I found to be highly effective too. The 2019 ACA Meeting Team were the Program Chairs: Stephan Ginell and Vivien Yee, both from the USA, and the Poster Chairs were Louise Dawe and David Rose, both from Canada.

The conference day zero had a suite of Workshops spanning nanomaterials, cryoEM, serial protein crystallography and powder diffraction in phase identification and materials characterisation as well as one on career development. The opening keynote presentation paid tribute to **Michael G Rossmann** (1930-2019), Pioneer in Crystallography of Macromolecules and Viruses. There were five speakers selected to cover the various decades of Michael's illustrious career in science. Chaired by **Janet Smith**, the speakers were **John E Johnson** of Scripps, **Eddy Arnold** of Rutgers University, **Hao Wu** of Harvard Medical School, **Rui Zhao** of the University of Colorado and **Saif Hasan**, Maryland School of Medicine. The special position that Michael held in our minds and hearts was reflected in these very warm tributes of the speakers.

There were Award Lectures, presented as per the ACA tradition at 8am in the morning, to launch each day of sessions. The Trueblood Award was to **Brian Toby** and **Bob von Dreele**, the Fankuchen Award was to **Ed Lattman**, the Bau Award was to **Bryan Chaukoumakos** and the Margaret C Etter Early Career Award was to **Efrain Rodriguez**.

As well as the buoyant poster sessions held each of the three days were a variety of events at lunchtimes or in the evenings. These were the 'First time attendee and student orientation', the 'Three minute thesis competition', the 'CCDC celebration of 1 million crystal structures' and the 'Dectris Young Crystallographer SIG Mixer'. There was also of course the ACA Business Meeting (which BCA would term the Annual General Meeting). Also the various SIGs held their meetings not least to canvass ideas for the ACA 2020 to be held in San Diego. Due to the close timing of this to the IUCr 2020 in Prague, due to a 'difficulty in finding suitable dates' for the ACA2020, the planned focus looks to be on 'education, American neutron, synchrotron and X-ray laser facilities and invitations to relevant American funding agencies'.

The day long ACA 2019 Transactions Symposium was entitled 'Data Best Practices: Current State and Future Needs' and in which I presented the opening talk. As Chairman of the IUCr's Commission on Data and as IUCr's Representative to CODATA I gave an overview of IUCr's roles and achievements in this domain. I included a short resume of the deliberations and recommendations of the IUCr's Diffraction Data Deposition Working Group which I chaired and ran from 2011 to 2017.

I also attended Microsymposia on 'Diffuse scattering for biological structure and dynamics', 'New toys: Light sources, beamlines and detectors', 'Time-resolved @ XFELS', 'Application of anomalous techniques in macromolecular crystallography', 'Radiation damage in X-ray crystallography and cryoEM' and 'What is the meaning of resolution?' I session hopped occasionally to hear eg 'Building the future of crystallography through active engagement' from **Amy Sarjeant** and **Suzanna Ward** of CCDC and 'How structural biologists and the protein data bank contributed to recent US FDA new drug approvals' by **Stephen Burley**, Director of the wwPDB. My questions and observations in one of the sessions were described as 'feisty', spanning radiation damage and metals as well as the need for experimental evidence of two protein subunits coming apart, 'really?'. I quizzed a cryoEM speaker over coffee about the challenges to cryoEM to locate and identify metals and therefrom the importance of complementarity with X-ray anomalous dispersion methods and neutron crystallography to give room temperature, damage free, with hydrogens, structures.

There were some unavoidable clashes. I would have really liked to attend the Microsymposia on 'Cutting edge cryoEM', 'Microcrystal electron diffraction', the Structural Dynamics journal's 'Structure without structure', 'Locating and refining H atoms using X-rays, Neutrons and Solid state NMR', 'Structural biology combining solution SAS and high resolution methods (cryoEm, MX, NMR)', 'Diversity and Inclusion-Diverse Teams Perform Better' and 'Sustaining Crystallography Education and Training'.

I helped with the judging of the Pauling Poster Awards. I had to swap from chairing the judging of the Structural Dynamics Posters whose session clashed with the ACA Fellows' Reception.

There was a very interesting Vendor Exhibition. Oddly this was closed at lunch time and was separated from the lecture rooms, being one floor below. Coffee breaks were however in the Exhibition and Poster area.

With a packed program there was little time for venturing out. I did however enjoy a couple of evening meals out in Covington, a delightful village style area, as well as across the Ohio river in downtown Cincinnati for a USA style 'fish and chips'; I must remember to order the children's portion next time. My morning started pre breakfast taking advantage of the splendid Marriott Hotel 25m swimming pool, happily managing 1km each morning.

John Helliwell
University of Manchester

THE ACA annual meeting was held this year in Covington, Kentucky, which is just across the Ohio River from Cincinnati, Ohio. The ACA had previously visited Covington in 2003. An oppressive heat wave greeted us on Saturday morning, with temperatures eventually topping out in the high 30s and nearly 100% humidity. Luckily the indoor weather was more hospitable.

The format for the ACA annual meeting has varied in the last decade to best match attendance and reduce parallel sessions with overlapping interests. This year the meeting was four full days of sessions, preceded by a warm-up day containing workshops, an opening keynote and reception, and closed with a banquet on the last evening.

There were a number of workshops, one on career development, as well as many on technical topics ranging from structural characterization of nanomaterials and materials, software for cryo-EM analysis, to serial crystallography. I participated in the "Accelerating Your Career Development" workshop as one of the career mentors. There was a panel discussion followed by a mentor-mentee speed-meeting session. I enjoyed speaking with a number of students and post-docs, and answering their questions about life at a synchrotron, potential experiments and life in science in general.

The opening evening keynote was a group affair, in memory of **Micheal Rossmann**. Led by **Janet Smith**, the 6 speakers shared scientific insights and touching memories. Following this moving session, we adjourned to the exhibition hall for drinks, snacks and the hive-mind determination of which vendors brought the best swag; Dectris never fails with their scrumptious Swiss chocolates, but the CCDC always draws a crowd with their ingenious algorithms for crystallographic competition.

Each day of sessions started with a plenary – the first morning opened with **Brian Toby** and **Bob Von Dreele** receiving the Trueblood award for their work on GSAS and GSAS-II. They both spoke, sharing technical wisdom as well as enjoyable anecdotes. The ACA schedule is generally a hectic affair full of late nights, and I have to confess that I rarely make it to the 8am plenaries, but this pair of awardees was worth the effort. Their presentations were recorded and will be available on the ACA website in the near future.

Later Sunday morning, I was ensconced in the Crystallography in the Geosciences session, run by **Nichole Valdez** and **Caleb Chappell**. **Shaunna Morrison**, of Carnegie GPL detailed the challenges of doing diffraction on Mars with the Curiosity rover. Sunday afternoon, I had the privilege of chairing a session on Crystallography at Extreme Conditions, which had a diverse slate of topics. **Fahima Islam** from Oak Ridge shared the process of creating a 3D printed collimator for high pressure neutron experiments, using machine learning. **Richard Gillilan** from CHESS described his SEC-SAXS beamline, which subjects samples to deep ocean pressures. **Angus Wilkinson** (Georgia Institute of Technology) recounted his adventure with high pressure studies of perovskites, in which the helium pressure medium decided to assume a more prominent role within the sample structure. **Branton Campbell** shared a reversible topotactic transition of CsCoO2 at high pressures.

Sunday evening featured competing vendor events, Bruker vs Rigaku, which strongly polarized the community. Some adventurers attended both – Rigaku for drinks, Bruker for food, drinks and live music. I personally didn't feel like braving the elements and venturing the couple of blocks to the Rigaku event, so I crossed the street to the Marriott and partied with the Bruker folks. The Eskimo Brothers, a three piece band from Nashville, thrilled the Bruker event crowd with their virtuoso skills on their instruments, and faithful reproduction of country and rock hits. A good number of prominent crystallographers unveiled their dance moves, as a sneak peek of what was to come at the closing banquet.

For some mystifying reason, many of us weren't at our most spry on Monday morning, but interesting talks lured us back into the conference center. I spent my morning at the session with the intriguing title "What is a Crystal, in Time & Space." **Larry Falvello** shared some historical and contemporary thoughts on the definition of a crystal and crystal structures. **Stephen Byrn** detailed how X-ray pair distribution function (XPDF) methods have been illustrative in crystalline and amorphous samples. **Sean Barrett** gave a talk about time crystals that was enjoyable, but maybe more physics than most of us were ready for on this morning. At this point I scurried out of the meeting room – one difficulty of being involved with scientific interest groups in the ACA are the troublesome lunchtime meetings. I had two parallel meetings to attend, so had decided to venture out early for sustenance. My go-to place during the ACA meeting was a local chain called Lee's Famous Recipe fried chicken. The sides were ho-hum, but the chicken was perfectly breaded and cooked to succulent perfection. It was a 5 block walk, sometimes in spitting rain, but completely worth it to be attending lunch meetings as the envy of my hungry colleagues.

As any attendee knows, the best laid plans of session attendance fall by the wayside during the actual conference. I was confronted with numerous interesting sessions running in parallel. General Interest, which is usually a catch-all session for talks which don't fit any of the themed sessions, had a strong representation of interesting chemical crystallography talks. **Suzanna Ward** of the CCDC discussed the recent deposition of the millionth structure in the CSD, and the implications of this milestone. **Carol Brock** detailed the approximate symmetry than can exist in Z'>1 P1 structures. **Kevin Gagnon** of Vertex explained the dreaded chiral solid-solution, which he faced when optimizing pharmaceutical crystallizations. Day three presented even more conflicts between sessions, with supramolecular chemistry returned to the ACA, but competing directly were two interesting sessions: Functional Sustainable Materials and Home-Built Software and Hardware. I attempted to superposition myself, but eventually had to accept that my attention span wavefunction wasn't up to the task. **Christer Aakeroy** and **Tomislav Friscic** reinforced their status as perennial favorites. **Richard Cooper** shared his recent program HUG which, when coupled with SQUEEZE, improves the quality of an absolute structure determination, when solvent has been removed.

Richard Cooper (Oxford) presenting on the CRYSTALS software

Richard should also be commended for his use of memes and pop-culture references in the name of science i.e., Aliens, crystallography style: "In space, no one can hear you resonantly scattering." **Martin Ward** gave an enjoyable and in-depth description of the various tools in the high-presssure practicioner's tool-box, including X-rays, neutrons and computational studies. He also shared a technique from his recent CrystEngComm paper, where he used an anti-solvent to assist high pressure crystallization.

After that packed full day of sessions a great talks, many in the chemical crystallography community remained, buoyed by the promise of ugly structures and free food, for the much loved session, "Would you publish this?" Among others, **Stacey Smith** shared some misbehaving twinned data, **Richard Staples** described his troubles determining chirality from synchrotron data, and **Brandon Mercado** showed how a little help from his friends got him through some CheckCIF struggles.

Brandon Mercado (Yale), Marilyn Olmstead (UC Davis) & Christine Beavers (Diamond Light Source)

Wednesday, the final day of the conference, arrived packed with sessions competing for chemical crystallography attendees. "Cool Structures," the traditional forum for exciting, complex or scientifically outstanding chemical crystallography, was expanded to a full day from the typical half. This conflicted with an in situ and in operando measurements session, a crystallographic education session in the afternoon and a diversity and inclusion session in the morning, which had previously been run at ACA meetings in the evenings but benefitted this year from the more expansive time slot.

After this whirlwind of sessions, it was finally time to put on those dancing shoes, meet up at the shoreline below the hotels and board the Queen of Cincinnati for the closing banquet. In the last couple of years, the banquet ticket has been included in the registration of the conference, which has greatly improved the attendance, ambience and entertainment of the recent banquets. After dinner entertainment was provided by Cincinnati band, the Trailer Park Floosies, who provided a rollicking atmosphere of danceable tunes until midnight.

The ACA 2020 planning meeting occurred the following morning, and a strong program has grown around the theme of "Educating the next Generation." The 2020 program chairs are **Carla Slebodnik** (Virginia Tech) and **Nozomi Ando** (Cornell). Sessions and workshops on techniques, data validation, and research opportunities at central facilities have all made the provisional program. ACA 2020 will be held in San Diego, CA, on 1-6 August.

Christine Beavers
Diamond Light Source

(Photos courtesy of Christine Beavers)

The CSD Leaderboard

Covington by day

Covington by night

Getting Involved in the IYPTCrystals Project

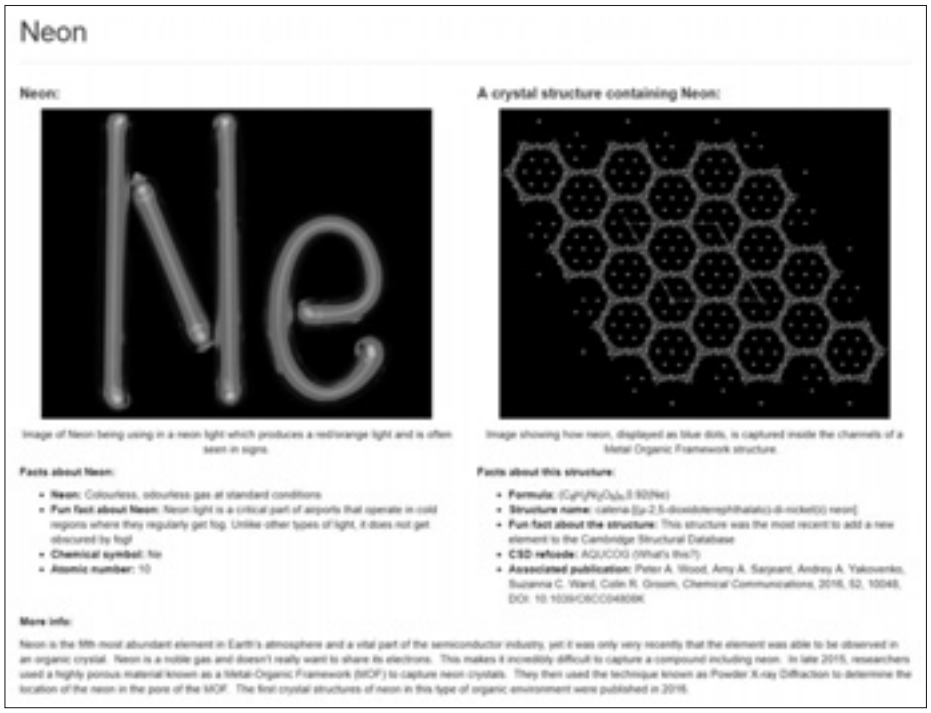
ARE you keen to help share the wonders of the periodic table and crystallography to a new generation of scientists? If so, we might have the perfect opportunity for you!

The United Nations declared 2019 the International Year of the Periodic Table.[1] "The IYPT 2019 is an opportunity to reflect upon many aspects of the periodic table, including its history, the role of women in research, global trends and perspectives on science for sustainable development, and the social and economic impacts of this field."[2] Many scientists and scientific institutions are celebrating the IYPT and helping others learn about one of the most significant achievements in science with a variety of events and projects. Not wanting to miss this opportunity the CCDC and the BCA bring you the IYPTCrystals project, to celebrate the IYPT in crystal style![3] The IYPTCrystals project aims to collate information about each element and an associated crystal structure allowing people to see inside those crystals and to celebrate the amazing science that has been made possible through crystallography and the periodic table.[4]

This is a community driven initiative, so we are looking for volunteers to help contribute to the project. If you would like to write some information about an element and a crystal structure containing or related to an element, please email us. Not only will you be helping to communicate science, you will also be featured on our "Contributors" webpage.[5] An example featuring the element Neon is shown below. We are also working to help others use this resource in education by creating additional worksheets and educational material based on these pages. So, if you would like to help us expand our collection of educational material based on the IYPTCrystals project to be made available for schools, science festivals or uniform groups we are looking for volunteers to help with this too. Together we can help inspire a new generation of crystallographers. Please contact us by emailing hello@ccdc.cam.ac.uk.

Caroline Davies and the IYPT in Crystals Project Team (**Claire Murray**, **Simon Coles**, **Amy Sarjeant**, **Ben Littlefield**, **Suzanna Ward** and **Caroline Davies**)

Twitter: @IYPTCrystals



Example of an element webpage (https://www.ccdc.cam.ac.uk/Community/educationalresources/PeriodicTable/Neon)

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1. https://www.iypt2019.org/.
2. http://www.unesco.org/new/en/brasilia/about-this-office/prizes-and-celebrations/2019-international-year-of-the-periodic-table-of-chemical-elements/.
3. https://twitter.com/IYPTCrystals .
4. https://www.ccdc.cam.ac.uk/Community/educationalresources/PeriodicTable/.
5. https://www.ccdc.cam.ac.uk/Community/educationalresources/PeriodicTable/contributors/.

Big Data leads the way for Structural Chemistry

… STOP PRESS … STOP PRESS … STOP PRESS … STOP PRESS …

Press release

THE Cambridge Structural Database reaches one million structures, leading the way in structural data to inform drug discovery and materials development

Cambridge UK, 6 June 2019.

CCDC (The Cambridge Crystallographic Data Centre), world-leading experts in structural chemistry data, software and knowledge for materials and life science research and application, today announced a huge milestone for structural chemistry with the addition of the millionth structure into the Cambridge Structural Database (CSD).

The CSD is the world's repository of highly curated experimentally determined organic and metal-organic crystal structures. It is used globally by scientists in over 70 countries to understand how molecules behave and interact in three dimensions in the solid form and ultimately how this affects physical properties.

As the interest in 'Big Data' continues to grow in a time where machine learning and automation are changing the way pharmaceutical, agrochemical and many other industries work, reaching such a significant milestone is a huge achievement for the CCDC and the wider scientific community that contribute to and rely on this resource.

Large volumes of data such as this enable scientists to generate more replete answers from a more complete and diverse volume of information, ensuring confidence in the insights being drawn from the data. Furthermore, CCDC's focus on ensuring the integrity of the data within the CSD through stringent quality assurance and control steps adds even more value and confidence that scientists are obtaining the highest quality information to inform their research.

This rich data resource, alongside advanced search, 3-D data mining, analysis and visualisation software from CCDC enables scientists from both industry and academia to further their research and predict new outcomes. In addition, knowledge derived from the CSD underpins computational chemistry and molecular modelling and is relied on by industry for the development and manufacturing of new drugs and within academia to teach chemistry.

Dr Jürgen Harter, **CEO of CCDC commented**, *"This is truly an important milestone not only for CCDC but also for the wider scientific community. In addition to the value that lies in large sets of data like this to help scientists inform their research and decision making, we also pride ourselves on the high quality of the data, a result of the hard work of our expert in-house database team. Maintaining a policy of strict data interrogation ensures the value of the plentiful insights that can be drawn from the CSD, avoiding misinformation that can lead to wasted time, resources and ultimately cost."*

CCDC have announced the 1,000,000th structure to be a N-heterocycle produced by a chalcogen bonding catalyst activating multiple reactions steps sequentially. In the paper the authors describe a class of extraordinary chalcogen-bonding catalysts which enable the assembly of discrete small molecules leading to the construction of N-heterocycles in a highly efficient manner. The structure was determined by **Yao Wang** and co-authors from Shandong University in China and published in the Journal of the American Chemical Society (JACS).

"We'd like to congratulate Yao Wang and all of his co-authors, for publishing the millionth structure and we are so grateful to the 350,000 plus scientists from around the world that have contributed their data, enabling us to reach this milestone and placing CSD as the go-to resource for structural information within the scientific community", said **Suzanna Ward**, **Head of the CSD**.

Dr Wang commented *"We are delighted to hear that our structure (1-(7,9-diacetyl-11-methyl-6H-azepino[1,2-a]indol-6-yl)propan-2-one; CSD Refcode XOPCAJ) is the millionth structure to enter the CSD! We have used the CSD for over ten years because it is an excellent platform to report new crystal structures and an outstanding database to find inspirable chemical structures. It is a valuable resource to us and to many other scientists around the world so we are very proud to be associated with this milestone for the community."*

Peter Stang, **Editor-in-Chief**, **JACS**, **said** *"We are delighted to hear that the millionth structure in the CSD was published in JACS. We know our readers value the CSD as a trusted repository of structural data and some of our authors have demonstrated how this rich resource can accelerate scientific research. Our continued collaboration with the CCDC helps make this wealth of data more accessible to the community as well as helping us ensure the integrity of data published in our journals and we are proud to be associated with such a significant milestone in structural chemistry."*

When asked what's next for the CSD, Dr Harter commented that although the use of the CSD in the pharmaceutical and agrochemical industries is already well-established, it is now fast becoming a fundamental resource for research into new materials such as batteries, paints, pigments and dyes, and in particular the development of gas storage frameworks and

tailored catalysts. As environmental contamination and sustainability become increasingly important there is considerable potential on a global scale.

CCDC have noted a consistent rise in deposits from research taking place in China over recent years.

"It is an exciting time for life science and materials development research with markets such as China leading the way in scientific discovery. We are excited to see what insights we obtain from this market going forward" **Dr Harter commented**.

CCDC also have plans to further draw on insights and trends from the data to inform the direction of future research across different industries

For more information visit:
https://www.ccdc.cam.ac.uk/csd-1-million, or contact:
Lucy White at l.white@ccdc.cam.ac.uk.

About CCDC

CCDC are world-leading experts in structural chemistry data, software and knowledge for materials and life science research and application.

They are dedicated to the advancement of chemistry and crystallography for the public benefit. They specialise in the collation, preservation and application of scientific structural data for use in pharmaceutical discovery, materials development and research and education.

CCDC compile and distribute the Cambridge Structural Database (CSD), a certified trusted database of fully curated and enhanced organic and metal-organic structures, used by researchers across the globe.

Their cutting-edge software empowers scientists to extract invaluable insights from the vast dataset, informing and accelerating their research & development.

A Million Thanks to BCA Members!

NOW that the Cambridge Structural Database (CSD) contains one million structures we wanted to take this opportunity to thank you for helping structural chemistry reach this tremendous milestone. It seems fitting to reflect on some of the contributions from the BCA community as well as to highlight some crystallographers from the UK who very nearly authored the one millionth structure!

The sharing of one million organic and metal-organic crystal structures is an achievement of which we should all be extremely proud. Crystallographers worldwide have contributed to this achievement and BCA members have had a huge impact both in terms of the number of structures and the development of the CSD.

This milestone comes fifty-four years after work on the database first began. Its beginnings can be traced back to 1965 and two British scientists, namely **J.D.Bernal** and **Olga Kennard**, who had the vision and foresight that the collective use of data would lead to the discovery of new knowledge and that vision has certainly come true today. Many BCA members have had a significant influence on the growth of the CSD including the thousands of crystallographers who have published their data, past and present CCDC staff, and members of our Board of Trustees who have helped guide the development of both the CCDC and the CSD.

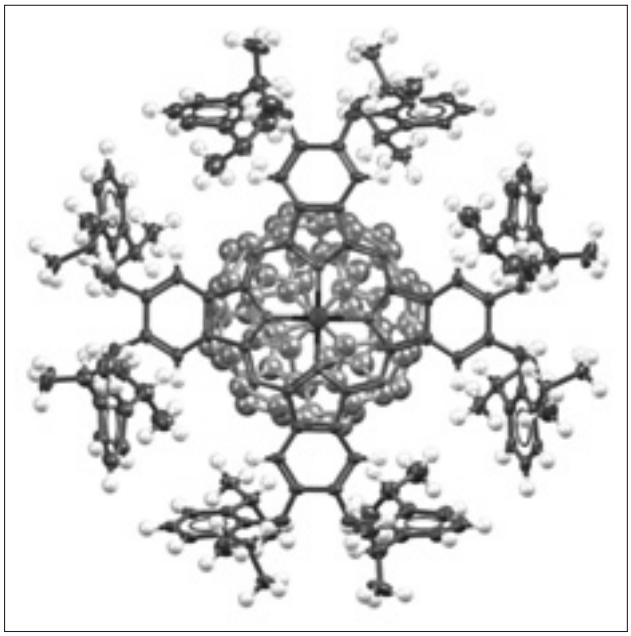
To date, the UK is an impressive sixth in the list of countries publishing the most crystal structures in 2019. Three of the top ten most prolific authors in the CSD of all time are from the UK, with **Mike Hursthouse** taking the fifth spot followed by **Alex Slawin** in sixth and **Judith Howard** in eighth. We owe our sincere thanks to these authors for their contributions and to all the other 350,000+ authors who have structures in the CSD.

continued >>>

A photo taken at Downing College during the CSD50 Event in 2015 showing some of the many crystallographers,scientists and CCDC staff and CCDC Trustees past and present who have contributed to the CSD over the years

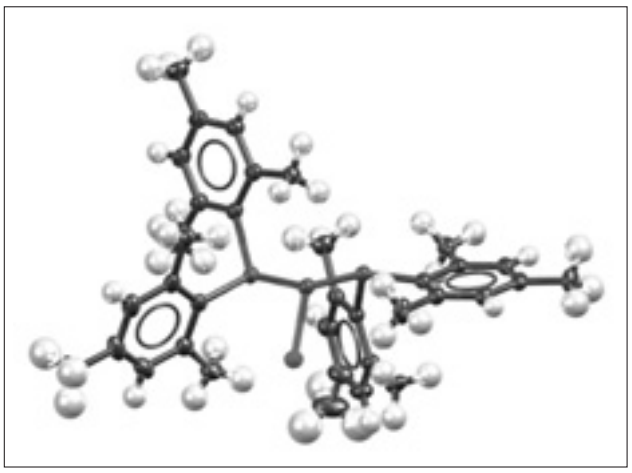
I am afraid a BCA member didn't quite get to author the millionth structure. I am, however, delighted to report that the millionth structure was determined by **Yao Wang** and his team from Shandong University in China – CSD Refcode XOPCAJ[1]. Perhaps somewhat surprisingly, none of the milestone structures listed on our stats page appear to hail from the UK, although the 900,000th structure does have a British author (CSD Refcode PATXEQ). With that in mind I thought it would be interesting to see how close the BCA community came to contributing the millionth.

On the same day that we reached one million structures, over 550 other structures were also published in the CSD. These were determined by over 170 different crystallographers from over 150 institutions. Out of those crystallographers a handful were listed as residing in the UK so a few of you were tantalisingly close to being the author of the millionth! On CSD one million day, nine crystallographers from seven UK institutions published 63 structures. The universities by order of the number of structures were Edinburgh, Manchester, Cardiff, Newcastle, Aberdeen and Bath. One publication from UK scientists dominated the list with a whopping 43 structures. So, **Stephen Moggach**, **Neil McKeown** and co-authors you nearly timed it perfectly, your structures on highly stable fullerene-based porous molecular crystals with open metal sites[2] were just a few structures away.



*CSD refcode KODVAD (DOI: 10.5517/ccdc.csd.cc204w8b) published by **Stephen Moggach and co-workers**[(2)].*

Unfortunately, I can't mention all the structures but some of the other UK crystallographers who nearly took the accolade were **Andrew White**, **Bill Harrison**, **Darren Ould**, **Jamie Purkis**, **Paul Waddell**, **Laurence Cook**, **Sultan Alkaabi** and **Zhen He**. Each one of the structures they published on CSD one million day is fascinating in its own right and also helps make the CSD the powerful resource of over one million structures that it is today.



*CSD Refcode XOLYOP (DOI: 10.5517/ccdc.csd.cc226t59) published by **Paul Waddell and co-workers**[(3)].*

For the curious among you we will be publishing a series of blogs on our website in the coming months highlighting some of the other structures that were published on CSD one million day. Keep an eye on our website and social media posts if you want to see which structures were in the mix and who were the other crystallographers so close to CSD one million![(4)]

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(1) Wei Wang, Haofu Zhu, ShuYa Liu, Zhiguo Zhao, Liang Zhang, Jingcheng Hao, Yao Wang, *Journal of the American Chemical Society,* 2019, **141**, DOI: 10.1021/jacs.9b03806.

(2) C. Grazia Bezzu, Luke A. Burt, Charlie J. McMonagle, Stephen A. Moggach, Benson M. Kariuki, David R. Allan, Mark Warren, Neil B. McKeown, *Nature Materials*, 2019, DOI: 10.1038/s41563-019-0361-0.

(3) Keith Izod, Peter Evans Paul G. Waddell, *Angewandte Chemie, International Edition,* 2019, DOI: 10.1002/anie.201905922.

(4) https://www.ccdc.cam.ac.uk/Community/blog/

Suzanna Ward
(Cambridge Crystallographic Data Centre)

BCA Industrial Group X-ray Fluorescence Meeting

Sheffield Hallam University, Wednesday 12th June.

IN 2018 the annual XRF meeting was held for the first time at Sheffield Hallam University. This meeting was a great success, so we returned to SHU in 2019.

45 delegates attended the meeting. 7 speakers gave talks at the meeting, including 3 from Germany! 12 exhibitors were part of a commercial exhibition and they all gave short presentations to advertise their wares as part of the Exhibitor Forum.

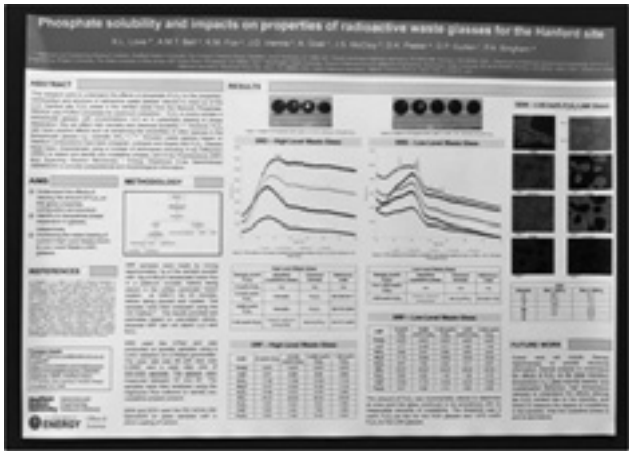
https://sites.google.com/site/bcaxrf/meetings/12-june-2019 gives full details of the meeting.

3 student places were taken up by postgraduate students from SHU. My Ph.D student, **Katrina Love**, kindly wrote a report on the meeting.

AMT Bell
Sheffield Hallam University

Annual XRF meeting 2019

FOLLOWING on from last year's event, the XRF meeting was once again held at Sheffield Hallam University and chaired by Dr Tony Bell. I was very kindly offered a student place and made great use of this opportunity to better acquaint myself with the theory and industrial applications of XRF. The little knowledge of XRF I did have had come from prior use during my undergraduate degree and currently in my PhD as a primary characterisation method to analyse my glass compositions.



My academic poster

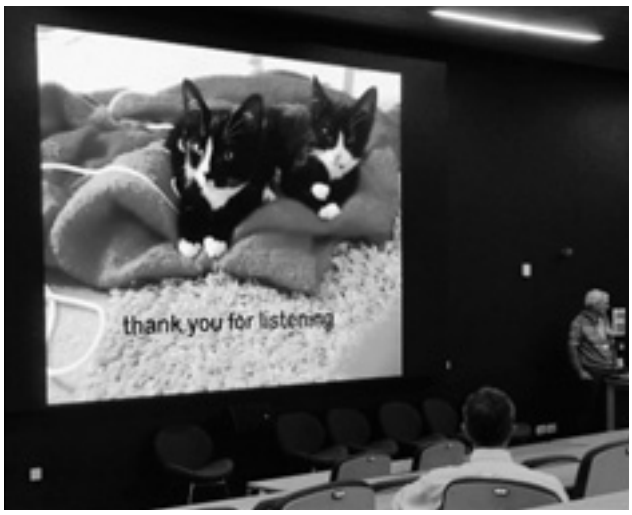
As I stepped through the revolving doors of the host venue, I made a bee line to the registration desk where my welcome pack awaited, personalised with my name printed on it. The main booth area was bustling with suit cladded bodies, rustling banners and teething with the sound of chitter chatter. It was incredibly interesting to see the equipment available from industry companies such as Bruker, FluXana and ATC to just name a few. There was XRF analytical equipment, preparation machines for grinding and pelletizing, and furnaces that make the fused bead samples. The equipment was more compact than what I was used to, with demo kits sitting idly on the provided stall tables.

The SciMed stall

The official welcome talk was given by **Dr Tony Bell** as he gave a whistle stop tour of what got him involved with XRF and how he had been using it. He described how he entered the world of XRF when a colleague had asked about the composition of a clay that contained silver. At that time the OXI method did not have a silver calibration standard, which led to Tony developing it at SHU along with other samples.

The day continued with 3-minute pitches from vendors informing the audience of their key findings and top equipment, then by specific talks where XRF had been used. Some of the talks that I found particularly useful and interesting included 'light element mapping by WD-XRF' by **Malcolm Haigh**, SciMed, 'The analysis of suspended particulate matter using ED-XRF' by **Andrew Scothern**, Malvern Panalytical and 'Biasing pitfalls in sample preparation for XRF analysis' by **Martin Lischka**, HERZOG Maschinenfabrik GmbH. These talks highlighted to me the scope that XRF can have and the impact of having smarter machines can

Tony Bell's opening talk



have for businesses. A few seconds quicker at grinding, pouring and releasing of samples saves a lot of time and money on the shop floor. I learnt that procedures in the lab that I take for granted when preparing my XRF sample powders, such as how I transfer my powder or pack it, can affect the results and errors I get.

Overall, while this year's meeting had a smaller number of attendees than last year, the quality of presentations was great and organisation was well established. It would have been nice for there to have been more posters evidencing use of XRF from industry and academia, hopefully this will be the case in the future.

Katrina Love
Sheffield Hallam University

The Erice Magnetic Crystallography School

I WOULD like to thank the British Crystallographic Association for the bursary, without which I could not attend the Magnetic Crystallography School in Erice, Italy. I also need to thank the organisers of the event who did so well to organise over 100 people arriving in the small mountain town of Erice at 750m above sea level, but also to pass on such valuable knowledge. The town of Erice looks out over Sicily and has history dating back to 400 BC, but now scientific meetings are held here fairly regularly on a variety of topics.

I arrived in Sicily ready to present my poster on 'Frustrated Magnetocaloric Frameworks' to the fellow attendees of the event. Our results have indicated that the combination of magnetic frustration with 1D ferromagnetic chains seems to greatly increase the efficiency of magnetocaloric materials. We have been attempting to optimise the magnetocaloric effect for temperatures below 20 K and in low applied fields, for the application of cooling superconducting magnets as an alternative to helium vapour compression refrigeration. Through neutron diffraction we have studied the short-range correlations and magnetic structure of some efficient materials of this type.

The study of frustrated magnetism takes traditional crystallographic techniques to the limit, as competing interactions prevent the formation of typical long-range order. In order to properly study and analyse this, it is essential to understand crystallography more deeply. The collection of expertise at this meeting made attending it crucial to the progression of my work.

To understand the average structure of these materials we apply the Rietveld technique and attending this event were the writers of some of the best software for this approach. Until this meeting I had questions about the ways in which the software works and had unsolved problems. I was introduced to new techniques and approaches to solving these problems and through speaking with the attendees I have left having learnt so much. One of the most interesting talks was from **Branton Campbell** at BYU, which gave a complete description of magnetic crystallography and whose research has helped many crystallographers. **Laurent Chapon** at Diamond gave a fascinating talk highlighting the use of X-rays for magnetic structure determination, which provides information not accessible through the typically used neutron techniques.

The event ended with some great talks from PhD students and a question panel for the event organisers about magnetic crystallography which was very insightful. My PhD is soon coming to an end and the skills, potential for collaborations and knowledge I left with will carry me to the end of my research and on to my next endeavour. Thankyou.

Richard Dixey
University of Kent

17th BCA/CCG Intensive Teaching School in X-ray Structure Analysis

THE 17th BCA/CCG Intensive Teaching School in X-ray Structure Analysis was held at Trevelyan College, Durham from the 6th April – 14th April 2019. The school had an international feel with just over a third of the 80 students being based outside the United Kingdom, from a total 15 different counties: UK, Argentina, Australia, Austria, Chile, Croatia, Finland, Germany, Ireland, Malaysia, Malta, Poland, Singapore, Spain and Switzerland. The atmosphere throughout the school was very friendly and supportive, which was noted positively in feedback from a number of the students and staff alike, with the variety of nationalities, different academic backgrounds and range of crystallographic experience creating an interesting environment both for learning and meeting new people.

The school has both a national and international reputation for providing a good basis in crystallography which meant that we were once again heavily oversubscribed. The format of the biennial course has evolved as a result of feedback from students and staff and currently consists of a mixture of lectures and tutorials designed to help students improve their understanding of the lecture material. The course, as the name suggests, is intensive with a full timetable across the 7 days providing the students with the opportunity to gain a good theoretical understanding of various aspects of crystallography from a single crystal perspective. Following an introductory lecture shortly after arrival the lecturers, Professor **Simon Parsons**, Dr **Lukas Palatinus**, Dr **Andrew Bond**, Dr **Helena Shepherd**, Dr **Richard Cooper** and Dr **Mark Senn**, guided the students through the following topics over the course of the week; Math, Symmetry, Data collection, Fourier/Patterson, Charge Flipping, Superspace, Direct Methods, Parameterisation, Least Squares, Refinement, Derivation of Results and Twinning. The tutorials are organised such that each of the participants is assigned to a tutorial group for the week that consists of 8 tutees and a tutor, who work together throughout the week to tackle a series of problems relating to the recent lecture material. This year we welcomed four new tutors: Dr **Christine Beavers**, Dr **Laszlo Fabian**, Dr **Claire Hobday** and Dr **Hamish Yeung**, as well as welcoming back Dr **Iain Oswald**, Dr **Andrew Cairns**, Dr **Nick Funnell**, Dr **Amber Thompson**, Dr **Claire Wilson** and Dr **Hazel Sparkes**. As usual the lectures and tutorials were held in the Sir James Knott Hall which enables us to switch easily between formal lectures and tutorial work with minimal disruption. The accommodation and meals were provided in Collingwood College which is less than a 5 minute walk away but provided a pleasant chance for some fresh air and brief exercise during the day.

As is traditional at the school, apart from the Math's lecture on the first day, the evening activities are designed to be more relaxed and provide an opportunity for the students to mix with each other through a combination of educational and fun activities. On the Sunday evening, a successful bar quiz, organised by **Richard Cooper**, resulted in a tight result with three of the teams being within one point of each other at the end. The Monday evening session provided an introduction to Databases (Dr **Pete Wood**) while the use of Synchrotron and Neutron facilities (**Christine Beavers** and **Mark Senn**) were highlighted on Tuesday. This year's student presentations, on the Friday evening, were organised by **Nick Funnell** and **Claire Hobday**. Each of the tutor groups put together a short (~5 minute) presentation on a crystallographic topic drawn from a hat earlier in the week in a style that was also chosen at random e.g. Local Structure in the style of the Bake Off, or

the Bravais Lattice in the style of Bear Grylls. All of the groups put together creative and amusing presentations on their respective topics which created an enjoyable evening with much hilarity. As with previous years the educational and entertainment value of each presentation was assessed by our elite panel of judges, the lecturers, who were very impressed by all of the entries.

The conference dinner on the Saturday evening provided the chance to thank all of the people who had contributed to the success of this year's school, the local staff, organisers, lecturers, tutors and students. The hard work and positive attitude from the staff and students alike all helped to create a very friendly school. After this year's school **Simon Parsons** has stepped down as scientific director, we would like to thank him very much for his contribution over the last 10 years. His enthusiasm and drive have helped maintain the high standards of the course while keeping up to date with current developments. We are delighted that Simon is staying on the lecturing staff for the next school and very pleased that **Richard Cooper** has taken over as the scientific director and wish him every success.

Following on from the school an optional hands-on Olex2 workshop was held on the Sunday, run by Dr **Michael Bodensteiner** and Dr **Oleg Dolomanov**. This was well received by the ~40 registered participants who had the opportunity to use Olex2 to apply structure solution and refinement concepts that they had learnt on the course to both test structures and their own data.

I would like to finish by saying thank you to all of the sponsors for this year's school which were Diamond, IUCr, ECA, CCG, IG, Oxford Cryosystems, Bruker, Rigaku Oxford Diffraction, Cambrex and the National Crystallography Service. Without the financial support from these organisations we would not have been able to help as many students attend the school or run it so successfully and we are very grateful for their continued support.

Hazel Sparkes
Local Organiser

CCDC Annual Science Day

CCDC
advancing structural science

CCDC held its annual Science Day on Friday 14th June. The event brings together a cross-section of industrial and academic scientists but is focussed around the current CCDC-sponsored PhD studentships worldwide. This Science Day gives each student an opportunity to showcase their ongoing work and gain feedback from their peers and from eminent scientists in the community.

This year, the Science Day was adjacent to CCDC's European UGM which gave the PhD students the opportunity to highlight their work to a broader group of industrial CCDC users through flash presentations of 2 minutes each the day before.

First up on the day was **Aurelia Li**. Aurelia, from the University of Cambridge, gave an interesting presentation on her work on porous materials (with a focus on Metal-Organic Frameworks). Porous materials are important for gas separation applications amongst other areas. Aurelia has worked with CCDC to develop a MOF subset of the CSD which now contains 93,000 structures.

Aurelia has worked on classification of MOFs in recent work, including characterisation based on MOF type and network dimensionality. She's developed a nice web visualisation for filtering MOFs based on properties and has recently been working on high throughput screening for hydrogen storage.

Matthew Reeves from the University of Edinburgh then updated us on his final year work on predictions of oxidation state of compounds in the CSD. During his PhD, Matthew has tackled the challenges of extracting oxidation state information and how to augment the CSD with such information. Matthew's approach uses the Bond Valence Sum (BVS) method alongside three ligand-based approaches to assign the oxidation state to a given structure. The BVS approach alone is quite successful for first row transition elements. For a more reliable and more generalisable workflow, Matthew has included additional approaches, such as calculating the maximum hardness using semi-empirical methods, to assign ligand charges which in turn can be used to infer oxidation state.

Matthew has put these approaches together into a consensus-based approach, generating an overall confidence score to oxidation state assignments. Using the assignments, a user can begin to deconvolute information from the CSD, such as the consequences of Jahn Teller effects on bon distances. Matthew has also developed a PIXEL interface for Mercury!

Alex Moldovan, University of Leeds, then spoke about his PhD on interfacial interactions between faceted crystals. Alex has created a modelling framework for surface-surface interactions. This works by bringing together excipient and API surfaces and assessing how the faces interact with each other. Alex has studied 3 compounds in contact with paracetamol and is able to understand how facet energies change across surfaces with rotation and translation of the other surface to identify surface cohesion and adhesion and the method can allow a user to understand the respective

properties of the system. More recently, Alex has used AFM to test the outcomes of the modelling experimentally.

In drug discovery, fragment-based approaches have become de rigueur in recent years. **Mihaela Smilova**, University of Oxford, told us about her project on working on using fragment hotspot maps for establishing selectivity of binding in pockets by compiling ensemble maps from aligned protein structures. Mihaela has looked at and solved the challenges of extracting information from the combined hotspot maps. She is exploring whether it is then possible to use these maps and identify selectivity regions. The program works well to identify the causes of selectivity in bromodomains for polar regions. The apolar maps seem to work well in kinases, and the method has been further validated using CK2alpha.

Conformations are also of key interest in drug discovery & drug development. **Sarah Wright**, University of Manchester, gave us an update on her project to understand the nature of conformation in crystals. Sarah uses two concepts, namely conformational change versus conformational adjustment. Sarah has developed a new way to classify torsion angles that are “unusual” (as defined by CCDC’s Mogul software) into different types of “unusualness”, the difference being where a local adjustment would lead to a usual torsion as opposed to where a molecule would need to rotate through an energy maximum to get to a usual torsion. Interestingly Sarah sees that, using her metrics, 30% of structures contain an unusual torsion using her newer finer grained definition. Next, she’s going see whether polymorphism can be sub-divided using the new metrics.

Many students are now taking advantage of machine learning for building of predictive models, and we heard a tranche of talks that showcased such approaches.

Jakub Janowiak, University of Leeds, told us about melting point predictions using message passing neural nets. Melting points are a part of solubility and allow us to understand the occurrence of "brick dust" crystals. Jakub has used 53,756 CSD structures with melting point information. He has encoded information from various sources that encode both molecule information and crystal information. Surprisingly, Jakub found little difference in models built on molecular information only as compared to crystalline information. Jakub has concluded, using polymorphs and matched molecular pair analysis, that chemical changes caused far higher changes in melting point.

Andre Frade, in his first year of his PhD at the University of Oxford told us about how he's developing methods to go from molecular to materials properties using machine learning with 2D molecular descriptors from RDKit. Andre is working on trying to predict formulation relevant descriptors for pharma. He has been developing a pipeline to achieve this going forward. Andre has included confidence thresholds in his approach so that any predictions can be assessed based on this. He chooses to only provide predictions where the model is at least 80% confident. This gives high accuracy but for a relatively small subset of inputs. He is applying his method to predicting hydrogen bond network dimensionality and to prediction of polymorphism.

Katerina Vriza, University of Liverpool, gave us an overview on her work on data-driven discovery of co-crystals. Firstly, Katerina gave us an overview of how you define a co-crystal and then told us why they matter in the pharmaceutical and electronic material industries. The project is aiming to design crystals specifically targeted towards superconductivity. Katerina has screened out two component systems from the CSD and removed all compounds with acidic hydrogens to create a dataset of 2000 suitable co-crystal pairs. is building multiple classification models to classify the dataset and has predicted some promising new co-crystal candidates.

Laura Straughair, University Strathclyde, told us about her efforts to predict solvated and hydrated forms. She gave us an overview of the methods currently available. She’s focussing on machine learning methods based on descriptors. She’s explored using molecular fingerprints as a descriptor (FCFP6) along with more traditional descriptors. This leads to a 77% success rate in prediction. She’s now moved on to experimental work for hydrate screening for new forms.

The final talk of the day was presented by **Victor Do Nascimento** from the University of Southampton. Victor gave us a tour-de-force show-casing his work towards using crystal structure prediction for hydrate prediction. He gave us a nice overview of why hydrates form, including an overview of how some drugs such as cefixime can lose efficacy due to hydrate formation. Victor is making predictions of hydrate formation using new CSP approaches with a newly parameterized energy model. He tries to find promising anhydrous structures in a crystal structure landscape that have sufficient space to accommodate hydrate molecules in cavities. He has managed to get promising predictions for some small rigid biologically relevant compounds.

Overall, we had a fantastic day with many stimulating presentations and plenty of time for discourse. We are already looking forward to next year’s event.

Jason Cole
CCDC

Obituary

Bill Town passed away on June 24th 2019.

BILL obtained a PhD in X-ray crystallography from Lancaster University and after graduating moved to Sheffield to research chemical structure search systems. Bill then worked in Cambridge with Olga Kennard from 1969 to 1974 helping to computerise the Cambridge Structural Database (CSD). This work led to the publication of the Molecular Structures and Dimensions book series in the early 1970s enabling scientists to more readily retrieve and discover published structures. After his time in Cambridge Bill went to work in Italy before founding Hampden Data Services in 1983 which was instrumental in developing many software products including STN Express. He then worked in Derwent Information Ltd and also ChemWeb which was ahead of its time as an early pioneer of a pre-print service for chemistry.

In 2002 Bill set up Kilmorie Consulting which, in partnership with his wife Maggie, went on to become Kilmorie Clarke Ltd whose activities include corporate video and conference production. Bill remained an active member of the chemical information community taking on a number of roles in the ACS Division of Chemical Information (CINF). In 2003 he returned to his crystallographic roots and became a member of the CCDC's Board of Governors serving for 9 years, helping to steer the organisation as Chair between 2005 and 2009.

Bill contributed an enormous amount to the CCDC and he will be very fondly remembered by staff past and present. Many of us will remember him for his gentle kind nature, his enthusiasm for travelling and eclipses (often both!), and his passion for politics and the European Union. Bill contributed greatly to both science and society – he will be sadly missed.

Bill's wife Maggie has set up a JustGiving page to raise money for the British Lung Foundation in his memory because Bill believed everyone should breathe cleaner air – https://www.justgiving.com/fundraising/maggie-clarke.

Suzanna Ward and **Ian Bruno** (CCDC)

AT the time of going to press we learnt the sad news that our colleague and long serving *Crystallography News* Editor, Carl Schwalbe, passed away suddenly after a very brief period in hospital. Our thoughts and best wishes go out to his family at this time.

CV

- **The CCDC**
- **2010-2019** Emeritus Research Fellow
- **Aston University**
- **2010-2019** Emeritus Professor of Medicinal Chemistry
- **2007-2010** Professor of Medicinal Chemistry,
- **1979-2007** Senior Lecturer in Medicinal Chemistry,
- **1972-79** Lecturer in Medicinal Chemistry
- **Max Planck Institute for Experimental Medicine**
- **1970-72** Research Fellow, (PI, Prof. W. Saenger)
- **Harvard University**
- **1965-70** PhD., (PI, Prof. William N. Lipscomb)
- **1964** AM
- **Oberlin College**
- **1959-63** AB, Chemistry (summa cum laude)

Carl and Joan Schwalbe at the 2009 ACA meeting (photo courtesy of Bill Duax).

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, news@crystallography.org.uk . Assistance from the IUCr website and the *Journal of Applied Crystallography* is gratefully acknowledged.

29 August – 4 September 2019
CIFiesta. AIC International Crystallography School2019, Naples, Italy.
http://www.cristallografia.org/aicschool2019

1-7 September 2019
CCP4/BCA Protein Crystallography Summer School, York.
https://synergy.st-andrews.ac.uk/proteincrystallography/

2-6 September 2019
1st International Conference on Non-Covalent Interactions, Lisbon, Portugal.
http://icni2019.eventos.chemistry.pt/#page-top

2-6 September 2019
Neutrons and Muons for Magnetism, Ispra (Varese), Italy.
http://www.sisn.it/nmm19/

2-12 September 2019
EMBO practical course on Image Processing for cryo EM, London.
http://meetings.embo.org/event/19-cryo-em

2-13 September 2019
16th Oxford School on Neutron Scattering, Oxford.
http://www.oxfordneutronschool.org/

2-13 September 2019
23rd Laboratory Course on Neutron Scattering Jülich & Garching, Munich, Germany.
http://www.fz-juelich.de/jcns/EN/Leistungen/ConferencesAndWorkshops/LabCourse/_node.html

7-20 September 2019
3rd Nordic-Baltic School in Neutron Scattering, Tartu, Estonia.
https://indico.nbi.ku.dk/event/1253/

8-14 September 2019
Fourth International School on Aperiodic Crystals, Cabourg, Normandy, France.
https://isac4.sciencesconf.org/

12-14 September 2019
HEC22. 22nd Heart of Europe Bio-crystallography Meeting, Obergurgl, Austria.
https://hec22.i-med.ac.at/

16-18th September 2019
International Conference on Materials Science and Engineering, Melbourne, Australia.
https://www.materialsconferenceaustralia.com/

16-20 September 2019
Neutrons for membrane biophysics, Garching (near Munich), Germany.
www.fz-juelich.de/jcns/SINE2020

23-25th September 2019
ESRF-EBS Workshop Series: Emerging Synchrotron Techniques for Characterisation of Energy Materials and Devices, ESRF, Grenoble, France.
http://www.esrf.eu/home/events/conferences/2019/energy-materials-workshop.html

23-27 September 2019
EMBO Practical Course: Small Angle Neutron and X-ray Scattering from Biomacromolecules in Solution, Grenoble, France.
http://meetings.embo.org/event/19-small-angle-scattering

24-25th September 2019
International SAXS Symposium 2019: SAXS excites, Graz, Austria.
https://www.anton-paar.com/tu-graz/saxs-excites

1-6 October 2019
Hot Topics in Contemporary Crystallography 4 Structural Biology, Dubrovnik, Mlini, Croatia.
http://htcc4.org/

1-6 October 2019
II School of the Latin American Crystallographic Association (LACA), Bucaramanga, Colombia.
http://ciencias.uis.edu.co/ivlaca2019/index.php

7-9 October 2019
EMBO Workshop: Tools for Structural Biology of Membrane Proteins, Hamburg, Germany.
http://www.embl-hamburg.de/training/events/2019/TBP19-01/

7-10 October 2019
1st French Congress on Integrative Structural Biology, Toulouse, France.
http://bsi-2019.ipbs.fr

7-10 October 2019
IV Meeting of the Latin American Crystallographic Association, Bucaramanga, Colombia.
http://ciencias.uis.edu.co/ivlaca2019/index.php

7-10 October 2019
JCNS Workshop 2019 Trends and Perspectives in Neutron Instrumentation: Probing Structure and Dynamics in Soft Matter, Tutzing, Germany.
http://www.fz-juelich.de/jcns/JCNS-Workshop2019

8-10 October 2019
Computational Approaches in Integration of Structural Biology Techniques. Instruct-ERIC workshop, Vestec near Prague, Czech Republic.
http://www.ibt.cas.cz/sd/udalosti/kalendar/191008-Instruct-ERIC-workshop.html

15-30 October 2019
CSHL X-ray Methods in Structural Biology Course, Cold Spring Harbor, NY, United States.
https://meetings.cshl.edu/courses.aspx?course=C-CRYS&year=19

17-20 October 2019
6th International Symposium on Diffraction Structural Biology (ISDSB2019), Osaka, Japan.
https://isdsb2019.symposium-hp.jp

21-26 October 2019
2019 ILL Annual School on Neutron Diffraction Data Treatment, ILL, Grenoble, France.
https://workshops.ill.fr/e/FullProf_School_2019

24-26 October 2019
The 77th Annual Pittsburgh Diffraction Conference, Oak Ridge, TN, United States.
https://conference.sns.gov/event/78/

3-5 November 2019
PSDI2019. 27th Protein Structure Determination in Industry meeting, Hinxton, United Kingdom.
https://psdi2019.org/

3-9 November 2019
EMBO Course "Practical Integrative Structural Biology", Hamburg, Germany.
http://meetings.embo.org/event/19-integrative-structural-biology.

13-15 November 2019
eBIC's 2019 Cryo-EM Sample Preparation Workshop, Didcot, United Kingdom.
https://www.diamond.ac.uk/Home/Events/2019/Cryo-EM-Sample-Preparation-Workshop-2019.html

16-21 November 2019
Third Asia-Oceania Conference on Neutron Scattering, Ken-Ting National Park, Taiwan.
https://www.aocns2019.org/

19-22 November 2019
X-Rays and Matter, Domaine de l'Asnée, Villers-les-Nancy, France.
http://www.rayonsxetmatiere.org/

20-22 November 2019
GISAXS 2019, DESY, Hamburg, Germany.
http://gisaxs2019.desy.de

1-6 December 2019
Advanced Materials Exploration with Neutrons, Boston, MA, United States.
https://mrs.org/fall2019/call-for-papers/call-for-papers-detail?code=MT04

9th Dec 2019 - 13th Dec 2019
American Geophysical Union Fall Meeting, San Francisco, CA, United States.
https://meetings.agu.org/fall-meeting-2019/

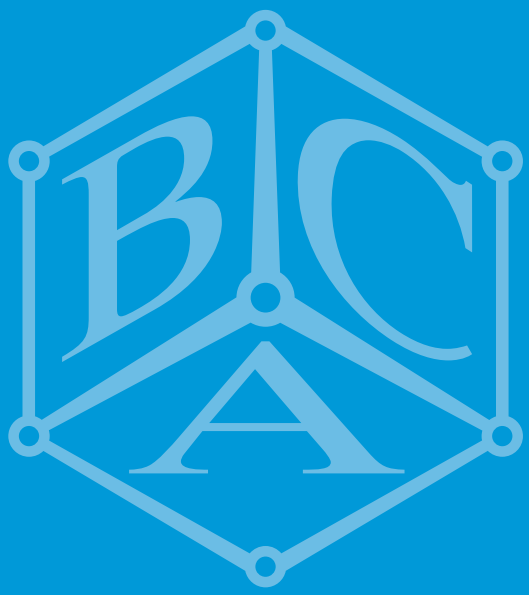
17-20 December 2019
16th Conference of the Asian Crystallographic Association (AsCA2019), National University of Singapore, Singapore.
https://asca2019.org/

26-28 February 2020
Materials Science & Nanotechnology Conference, Sana Malhoa Hotel, Lisbon, Portugal.
https://materialsconference.yuktan.com/

6-9 April 2020
British Crystallographic Association Spring Meeting, University of Leeds, UK.
https://crystallography.org.uk/spring-meetings/#next-meeting

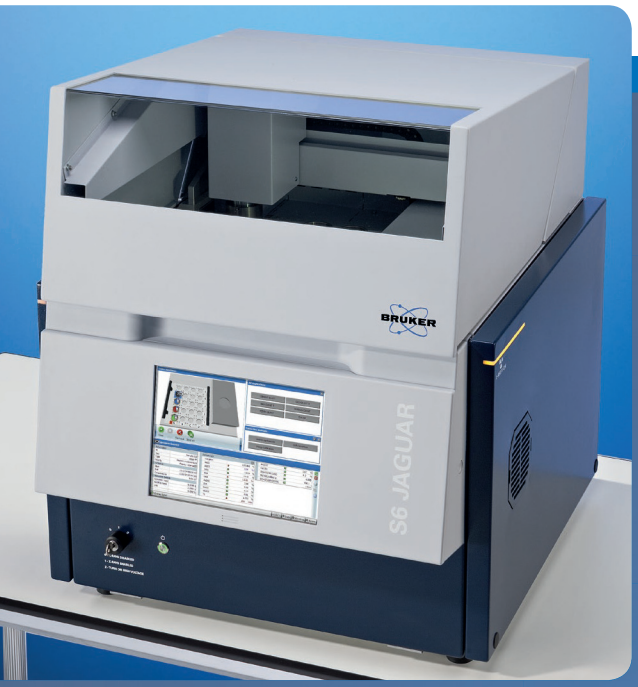
19-24 July 2020
Gordon Conference on Research at High Pressure, Holderness, NH, US, United States.
https://www.grc.org/research-at-high-pressure-conference/2020/

22-30 August 2020
Twenty-Fifth Congress and General Assembly of the International Union of Crystallography, Prague, Czech Republic.
http://www.iucr25.org/



S6 JAGUAR

Elemental Analysis with WDXRF in benchtop size



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