

16th BCA/CCG Intensive Teaching School in X-ray Structure Analysis

25th March – 2nd April 2017 Durham, UK



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25th March- 2nd April 2017, Trevelyan College, Durham, UK

Photograph courtesy of Dr Horst Puschmann, Olexsys

The 16th BCA/CCG Intensive Teaching School in X-ray Structure Analysis took place in Durham from the 25th March – 2nd April 2017. The school brings together students from a variety of countries, with different academic backgrounds and a range of crystallographic experience creating an interesting and friendly environment for meeting new people and learning. The 16th course was no exception being attended by 80 students who are studying or working in 16 different countries: the UK, Poland, Italy, Malta, Switzerland, Finland, Ireland, Brazil, Malaysia, Chile, Croatia, Germany, India, Uruguay, Saudi Arabia and Singapore. The majority of the students attending were PhD students with a small number of PDRA's and academic/industrial researchers all keen to learn more about crystallography. The national and international reputation of the school for providing a good basis in crystallography meant that we were once again heavily oversubscribed.

The course runs biennially and has evolved into its current format as a result of student and staff feedback as well as developments in equipment or methodologies which have also influenced the material covered. The course consists of a mixture of lectures and tutorials during which tutor groups work together to tackle a series of problems, each group consists of 8 students and a tutor who acts as a first port of call to help the students during the week. This year we welcomed two new tutors Dr Andrew Cairns and Dr Nick Funnell. The lectures and tutorials were held in the Sir James Knott Hall at Trevelyan College, which is an ideal space for the school allowing a quick switch between formal lecture presentations and tutorial work with minimal disruption. While the accommodation and

meals, which were of a high standard, were provided less than a 5 minute walk away in Collingwood College.

During the 7-day course the students were once again guided through the various aspects of crystallography following on from an introductory session (Professor William Clegg) lectures were given in the following order Maths (Dr Lukas Palatinus), Symmetry (Professor William Clegg and Dr Stephen Moggach), Data Collection (Dr Helena Shepherd), Fourier Synthesis and Patterson (Professor William Clegg and Dr Stephen Moggach), Charge Flipping and Direct Methods (Dr Lukas Palatinus), Parameterisation and Least Squares (Professor Simon Parsons), Refinement (Professor Richard Cooper), Derivation of Results and Twinning (Professor Simon Parsons). Each of the main sessions consist of a combination of lectures to introduce topics and tutorial exercises designed to help the students improve their understanding of the material. In addition, optional presentations on Superspace (Dr Lukas Palatinus) and Synchrotrons and Neutrons (Dr Mark Warren and Dr Mark Senn) were given and well received with essentially full attendance.

As is traditional at the school, apart from the Math's lecture on the first evening, the evening activities are designed to be more relaxed and provide a chance for the students to mix with each other through a combination of educational and fun activities. This year's course was no exception with activities including a bar quiz (Professor Richard Cooper), useful tips on crystallisation (Dr Dmitry Yufit), a talk on databases focusing on the CSD and associated software (Dr Peter Wood) and student presentations (Dr Katharina Edkins and Dr Helena Shepherd). As usual the student presentations were of a very high standard and provided a very amusing evening in which each tutor group presented a short play on a scientific topic in a certain theme both of which had been randomly chosen earlier in the week e.g. neutron diffraction as a musical or crystallisation in the style of a game show. The presentations were designed to be educational as well as entertaining and our elite panel of judges, the lecturers, were very impressed by all of the entries.

The conference dinner on the Saturday evening provided a chance to thank all of the contributors to the school, the local staff, organisers, lectures, tutors and students for helping to make it a very successful school. As this year's school marked 30 years since the courses started at Aston University in 1987, we were delighted to have four of the founding members present at the conference dinner Dr David Watkin, Professor Carl Schwalbe, Professor Bill Clegg and Professor Judith Howard whose enthusiasm and initial setting of the ethos have helped to make the school what it is today. Both Bill, as a lecturer, and Judith, as an organiser, have been associated with the school throughout the 30 years which is some achievement! To mark this Bill revived an old tradition and put together a school song describing events from the week in an amusing fashion, which he sang for us at the conference dinner to the tune of a Gilbert and Sullivan piece. However, Bill has decided to step-down from teaching at the school after this year's course and we will all miss his Escher T-shirts, wildlife pictures and jokes at future schools! Most of all though we will miss Bill's huge enthusiasm for teaching and communicating crystallography which along with his clear explanations and patience have benefited many students on the course over its 30 year history. Therefore, I would like say a huge THANK YOU to Bill for his enormous contributions to the school on behalf of myself, the school staff and all of the students who have attended the courses.

Following on from the success of the Olex2 workshop introduced for the first time after the previous school as a response to student feedback, Dr Horst Puschmann and Dr Oleg Dolomanov (OlexSys) ran another hands-on optional one day Olex2 workshop on Sunday the 2nd of April. This provided the 50 registered participants with a chance 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 and was very well received.

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, ICG, Oxford Cryosystems, Bruker, Rigaku Oxford Diffraction, CCDC and Pfizer. Without the financial support from these organisation 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.

ECA Support

The funds kindly provided by the ECA (€2000, £1697) were used to help the following students with contributions towards their subsistence.

Luke Frendo, University of Malta, Malta (£775)

Keith Flanagan, Trinity College Dublin, Ireland (£525)

Mladen Borovina, University of Zagreb, Croatia (£725)

Finally we would very much like to thank the ECA again for their financial support which assists with the running of this crystallographic school.

Professor Judith A. K. Howard, CBE, FRS and Dr Hazel A. Sparkes (Local Organisers)