

## **BCA/CCG Ninth Intensive Course in X-ray Structure Analysis**

**Trevelyan College, University of Durham, 7–15 April 2003**

The Ninth Course generally followed the successful format of its predecessors, but it continues to evolve to reflect developments in single crystal structure analysis. This year we increased the number of lecturers from four to five, with Simon Parsons the new recruit. We also had several new members of the tutoring staff. As in previous years the course was oversubscribed, even with an extra tutor group this year. This continued high demand shows how highly the Course is regarded by the crystallographic community both here and overseas.

The Course is based around lectures interspersed with tutorials in small groups of eight students: this time we had ten groups, a total of 80 students. The students came from a wide range of places, fields of study and backgrounds, and had a similarly wide range of experience of single crystal structure determination. Many of them were from overseas, including from Portugal, Denmark, Yugoslavia, France, Armenia, India, Finland and Ireland, and many other overseas students were already working in the UK. This gave the Course its typically strong international character. All lecturers and tutors are present for the duration of the Course, and available for informal questions or discussions: it is common to see tutors devote all or part of their coffee breaks to helping students with particular problems or queries. The immense skill, effort and commitment by the group tutors in engendering cooperation and collaborative working is a distinctive and vital part of the Course and, judging by student feedback, one of the most appreciated. This time we aimed to provide more support in the form of late-afternoon surgeries: it was intended that the lecturers provide these, but they were largely (and very effectively) used by students working within their own tutor groups.

The Course began on the first afternoon with some gentle introductions, including a reminder by David Watkin about some essential mathematics in the so-called “Matrix Mixer”. The Course continued for a further seven days with one much needed afternoon and evening off: it is intensive for everyone involved, but particularly for the students and tutors.

The Course covers all aspects of structure determination, including fundamental concepts of symmetry, diffraction, Fourier synthesis, direct methods, least-squares refinement and their application to solving and interpreting structures. The more practical aspects covered in lectures included topics such as crystal growth techniques, data collection, structure solution, refinement techniques and structural interpretation. The Course finished with two lectures given by staff of the Cambridge Crystallographic Data Centre: Owen Johnson on their new CIF editor, enCIFer, and Lucy Purkis on Mogul, the new knowledge-based library of intramolecular geometries derived from the CSD.

The evenings were given over not only to the Matrix Mixer, but also to sessions on crystallisation, a (partly crystallographic) bar quiz, an expert panel and student

presentations. In the last of these, each tutorial group worked to produce a science-based presentation, i.e a ‘performance’ of spoken word, singing or actions and these were all of a very high standard, hugely entertaining and surprisingly informative. One evening session was the Ceilidh, where dancing skills are optional. The Course Dinner took place on the final evening, where those responsible for making the Course a success – sponsors, organisers, lecturers, tutors, students and local staff – were all thanked for their efforts and everyone has a chance to relax after a very busy week.

The Course was clearly much appreciated by the students, who provided us with valuable feedback which will inform the content and structure of the next Course in 2005. There continue to be particular challenges in the wide range of previous experience of mathematics and crystallography. We are considering a number of ways to provide more support for the mathematical aspects of the Course. This year Peter Main kindly ran an impromptu session on essential mathematics, but in 2005 this should be a formal part of the introduction to the Course.

A book based on the Course, written by one past and three current lecturers and entitled “Crystal Structure Analysis: Principles and Practice” was published by OUP in late 2001 and has been very favourably reviewed. See <http://www.oup.co.uk/isbn/0-19-850618-X>.

The venue was again a highly successful element of the Course. Trevelyan College offers lecture facilities in close proximity to accommodation, catering and social amenities, so that different aspects of the Course can be smoothly integrated.

The number of scientists who depend on crystallographic structure determination continues to grow, as does the demand for structural results: it is an essential technique but one where they must acquire expertise quickly and alongside other methods. The Intensive Course is a unique resource, offering concentrated study and learning support not available elsewhere. Computational black boxes abound in crystallography. In many cases these work reasonably well with their default settings, but only by really appreciating how they work can difficult or non-routine problems be solved: developing this understanding is a prime objective of the Course. The Tenth Course is currently being planned, and will take place in Durham in April 2005.

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Sandy Blake  
University of Nottingham  
Course Director 2003