

Teaching crystallography through an intensive course

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Abstract. This contribution describes how an intensive biennial residential course has been developed to teach crystallography and structure determination.

Introduction

Almost twenty years ago we recognised that education in crystallography and structure determination was not receiving adequate in-depth coverage in many undergraduate and postgraduate courses, particularly in chemistry. Paradoxically, at the same time research productivity was increasingly underpinned by crystallographic methods. In 1987 a new course was held in Aston University, Birmingham and four more Courses followed there at two-year intervals, until the Course moved in 1997 to the University of Durham, which has now hosted three Courses. All of these have been residential and each has lasted approximately one week. The Course is intended primarily for young scientists at the postgraduate, postdoctoral or lecturer level who have some practical experience of structure analysis but who wish to improve their understanding of the underlying principles and practice. Although modern structure analysis systems enable routine structures to be determined with very little formal crystallographic training, such training is essential to ensure that the work is carried out competently and to allow problems to be identified and solved. It is also important to train crystallographic experts as leaders of the next generation.

Scope and organisation of the course

The Course aims to cover essential topics in the determination and analysis of non-macromolecular structures. These topics include symmetry, diffraction, crystal pre-

paration, data collection and reduction, Fourier syntheses, structure solution by direct and Patterson methods, refinement, structure evaluation and presentation of results. The aim is to cover the fundamental theoretical and practical aspects of structure determination and there is minimal reference to particular programs or packages. Although some use of mathematics is unavoidable, both the extent and the level are kept to a minimum. The Course now has five principal lecturers who cover the material, supplemented by eight or nine tutors, each of whom works with the same group of 8–10 students throughout the Course. The contribution of the tutors is vital and has been a major factor in the success of the Course. The timetable is arranged so that lectures and tutorials alternate through each day: each tutorial aims to support and expand on the immediately previous lecture and carry out worked examples directly related to it. Most evenings are a combination of the social and the educational: expert panels in the bar, crystallographic bar quizzes and student presentations by each tutor group. All the lecturers and tutors are present for the duration of the Course, and many students take advantage of this opportunity for informal questions to and discussions with the teaching team. The length of the course does not allow time for hands-on computer-based sessions, which would inevitably focus on the details of a particular package or collection of software at the expense of more fundamental understanding. We have found that the problem-solving tutorial style is far more effective for this.

Although most could be classified in some way as chemists, our students come from a wide range of backgrounds, including materials science, physics and biology. A significant fraction of students attending are from overseas, and this strengthens the exchange of knowledge and techniques between attendees on the Course. The formal and informal feedback we receive from the students and their tutors has been used to inform the content and structure of each subsequent Course. Some former students have returned to act as tutors on the Course and some former tutors have become lecturers. To date we know of some 20–30 graduates of the Course who are now in crystallography-related posts in academia and industry in the

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UK. Another lasting product of the Course has been a book [1] entitled "Crystal Structure Analysis – Principles and Practice" which was published by Oxford University Press and the International Union of Crystallography in December 2001.

The venue, Trevelyan College in Durham, plays no small part in the effectiveness of the Course: it offers all the necessary facilities for a residential course within a pleasant and stimulating environment.

The future

The Intensive Course is a vital resource offering a unique combination of concentrated study and extensive learning support. Its role will become even more crucial as the number of scientists involved in crystallographic structure determination continues to expand, but sadly the formal teaching at degree level has been reduced worldwide. It is essential that they acquire the necessary expertise. The

content of the Course is constantly evolving to reflect new techniques and practice. The future of the Course depends on having a suitable location, a dedicated team of lecturers and tutors willing to contribute a week of their time, and adequate funding. The first two seem assured but the third, as ever, is less certain.

The next Intensive Course will take place in Durham from April 7–14 2003. For further information contact Dr. Claire Wilson (E-Mail: Claire.Wilson@nottingham.ac.uk).

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Reference

1. Clegg, W.; Blake, A. J.; Gould, R. O.; Main, P.: Crystal Structure Analysis – Principles and Practice. Oxford University Press/International Union of Crystallography, Oxford, (ISBN 0-19-850618-X), (2001).