

MS23.01.05 X-RAY CRYSTALLOGRAPHY AND THE SYNTHETIC CHEMIST: "HANDS-ON" OR "HANDS-OFF"?

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X-ray crystallography is a powerful method for structure elucidation that should be one of the physical methods included in the education of contemporary synthetic chemists and materials scientists. The recent advances in area detector technology and user-friendly computer programs have reduced the time required to determine the structure of an organic compound to be competitive with multi-dimensional NMR experiments. In order for non-specialists to take full advantage of these advances, effective methods need to be available for novices to learn the essential fundamentals of x-ray structure determination in a practical "hands-on" environment. For several years we have offered a course which involves both lectures in crystallography and immediate "hands-on" experience on a research problem. A key to the success of this approach is the continued active involvement of the departmental crystallography facility and the staff crystallographer so that the students can move seamlessly from the course to using x-ray structure determination in their own chemical research problems. This presentation will summarize the evolution of the format of this course as instrumental and computing capabilities have changed. The use of interactive graphics programs and materials on the World Wide Web for teaching crystallography will be discussed, and approaches to developing an auto-tutorial program for introducing novices to practical x-ray structure determination will be described. The ever increasing importance of structural results to synthetic chemists and materials scientists requires that professional crystallographers and faculty develop facilities that can provide "hands-on" education in the powerful techniques of x-ray structure determination, as well as "hands-off" structural service.

MS23.01.06 TEACHING CRYSTALLOGRAPHY. WHO SHOULD BE TAUGHT WHAT? David Watkin, Chemical Crystallography Laboratory, University of Oxford, 9 Parks Road, Oxford, OX1 3PD, UK

A short while ago I was talking with an eminent chemist about the problems of teaching crystallography. She said, 'Isn't it just Bragg's Law and a few Fourier transforms?'. I stifled the reply 'Isn't synthetic chemistry just Alchemy with diminished expectations?', and began to explain that Bragg's Law and Fourier transformations were indeed fundamental, but for a practicing chemist, they might not be too important, since they were largely taken care of by computers these days.

In a recent article in 'Chemistry in Britain' (the news letter of the Royal Society of Chemistry) a writer explained how they had spent several years elucidating the absolute structure of an important natural product - not at the turn of the century, but recently - and without any reference to X-ray crystallography.

These two anecdotes illustrate some of the problems with teaching crystallography to the Wide World. Its common images, of being either too difficult or quite trivial, need updating and correcting.

MS23.01.07 TEACHING CHEMISTRY UNDERGRADUATES ENOUGH CRYSTALLOGRAPHY. Ward Robinson.

During the past 40 years the content of undergraduate chemistry courses has not changed greatly at the introductory level. This is evident if one examines dominant first year texts in inorganic, organic or physical chemistry. These traditional divisions of chemistry were all included in Linus Pauling's "General Chemistry" first published in 1947. Indeed those 710 pages also contain an introductory chapter on biochemistry and made minor but effective use of coloured diagrams. Present day popular texts are physically larger and use colour extensively and effectively but cover essentially the same material without which it is simply not possible to advance to the serious mastery of the subject expected of chemistry graduates. It is in this advanced study that we see enormous changes reflecting the stupendous wealth of new knowledge uncovered by chemists all over the world during a golden era in which many governments invested heavily in fundamental and applied research.

One consequence of this vast proliferation of factual material, not to mention the equally vast literature of conjecture the facts generate, is the competition for teaching time deemed the minimum essential by proponents of all the different facets of the subject including crystallography. The undergraduates still have only four years, at most, during which time they must be presented a balanced view of chemistry. Where does crystallography fit in and how much of it is essential?

One minimalist view of this will be presented. The perspective will be that of a chemical crystallographer with 30 year's teaching experience in a well equipped university but tempered by 10 years involvement in teaching programs in Asia where the perceived needs can be very different.

PS23.01.08 EDUCATIONAL ACTIVITIES OF THE BRITISH CRYSTALLOGRAPHIC ASSOCIATION (BCA). K.M.Crennell, British Crystallographic Association

BCA educational projects are described which have taken place since the last IUCr Congress; including a competition to design a crystallographic exhibit for an interactive science centre, a survey of educational software for microcomputers, a report on sources of educational materials to encourage young children to take an interest in crystallography and most recently, the setting up of BCA home pages on the World Wide Web (WWW) URL <http://www.cryst.bbk.ac.uk/BCA/index.html> where information on these projects is continually updated, together with news of forthcoming courses, meetings, job vacancies, links to journal publishers with contents pages, manufacturers and suppliers of crystallographic hardware and software.

The winning entry in the 'Design-an-exhibit' competition suggested the use of novel shapes of building blocks to show that space can be filled with models which are neither cubical nor rectangular. Photographs are shown of British children visiting 'Set95', the UK Festival of Science Week, trying the blocks. Planar nets of the shapes are also provided so that a class of children can try constructing cardboard models for themselves.

The report of the educational software survey for microcomputers was published in the June 95 issue of 'Crystallography News'; some results will be shown together with diagrams of screens from educational software, some of which is freely available over the Internet. This list is now on the WWW and is continually updated as readers send me information on their programs: newer programs have links to WWW sites where free 'demos' are available.

The BCA gratefully acknowledges support for World Wide Web activity from the Crystallography Department of Birkbeck College, University of London, and from the ISIS facility of the Rutherford Appleton Laboratory.