

Book Reviews

Works intended for notice in this column should be sent direct to the Book-Review Editor (R. F. Bryan, Department of Chemistry, University of Virginia, McCormick Road, Charlottesville, Virginia 22901, USA). As far as practicable, books will be reviewed in a country different from that of publication.

Acta Cryst. (1997). **A53**, 102

Structural electron crystallography. By DOUGLAS DORSET. Pp. xiii + 452. New York: Plenum Publishing Co., 1995. Price US\$ 69.50. ISBN 0 306 45049 6.

There can be few scientific subjects which have undergone such a revival and expansion of application in Materials Science in the past decade as Electron Crystallography, and in its application to the structure analysis of organic compounds Douglas Dorset has been a major contributor with an (unfinished) career spanning the period from 1974 to the present. The introduction of the term 'Electron Crystallography' to cover the dual-space studies of high-resolution imaging and electron diffraction possibly came from electron protein crystallography, but it is now more widely accepted in other material areas. The reader, however, should not expect a comprehensive coverage. Dorset, in his introduction, names the three major areas of application as inorganics, protein molecules and non-biological organic structures, but clearly indicates that his emphasis is on the third category, with only passing references to the other two.

With this restriction, the book gives a wide-ranging and clearly explained series of essays on precisely how to prepare samples, how to obtain data using low-dose microscopy and low-temperature stages and how to interpret the data, using various image enhancement devices and diffraction scan techniques, with the ultimate aim of solving the structural 'phase problem' for these compounds, many or even most of which are not amenable to X-ray diffraction because of their poor crystallinity.

Those sections of the book dealing with topics with which Dorset has been strongly involved are eminently readable, even for the lay scientist. For example, I found the history of the boric acid structure, with its detailed and easy to follow documentation (pp. 211–215) to be a fascinating insight into the contentious topic of the ability of electron diffraction data to provide *ab initio* solutions for structures. This quite apart from the occasionally heated debate about that particular structure – starting with Zachariasen in 1934, through Cowley (1953) and Craven & Sabine (1966) to Dorset, who in 1992 finally refined the structure to $R = 0.22$. Then again, who could fail to enjoy reading of the analysis, in the appropriate context of paraffins, of 'single crystals of wax from a child's birthday candle' (no colour is given: pp. 275–276).

On a more serious note, the whole thrust of this book is directed at the need to obtain 'quasi-kinematical' diffraction conditions, for which the loss of phase information is evident. In discussing inorganic structures (Chapter 7), the statement is made that 'Because of the complexity of the dynamic diffraction calculations ... the prevailing viewpoint is that *ab initio* structure analysis based on electron diffraction intensities or ... high-resolution micrographs is absolutely pointless'; and again, 'electron diffraction intensities are not simply related (to the structure) except in the case of dynamical extinctions

... if it were possible to find conditions (where this analytical method) could be applied to non-forbidden reflections it would be possible to use dynamic intensities ... in a simple way. Unfortunately ... this is not possible' (pp. 209–210). This kind of statement is unfortunate in a general context, since the dynamic calculations (for forward scattering) referred to are such that the symmetries of the crystal potential are preserved in the transmitted wave function, as was first pointed out by Cowley & Moodie (1957–1959). Dynamic extinctions are a consequence of sets of antiphase structure factors and there is a direct correspondence to this in those non-forbidden reflections affected by sets of in-phase structure factors, such as those lying along 2-fold diads or mirror planes.

However, the main interest in this book is with regard to the analysis of molecular organic structures, and it is here that Dorset makes a strong case for the early structural studies carried out by the Moscow school, which he says have been 'unfairly criticised by the crystallographic community'. It is true that in the period of development of dynamic scattering ideas in the 1950's and 60's many Western crystallographers attending international conferences would give little credence to structures derived from oblique texture patterns by applying only the Blackman two-beam dynamical correction to certain strong reflections. Nevertheless, in an extensive discussion of thiourea, which exists in both paraelectric and ferroelectric forms, Dorset shows that, in a refinement carried out by him in 1992 using the tangent formula of Karle & Hauptman, only 9 of the original 187 phases determined by Dvoryankin & Vainshtein (1960) required revision in the case of the paraelectric phase, while for the noncentrosymmetric ferroelectric phase the mean error in phase angle in the 1962 Dvoryankin & Vainshtein determination was only 11.5° . In both cases, it is claimed dynamic scattering did not seriously compromise phase determination. This example, however, also shows the enormous amount of labour needed to arrive at solutions for these organic molecules as compared with the more robust and better crystallized inorganic structures.

The book finishes with a brief review of the recent work of Henderson and others in the elucidation of globular protein structures. This is a field in which electron crystallography has led the way, owing to the extreme difficulty of obtaining sufficiently well crystallized samples for X-ray study.

This book will complement other recent publications in related, mainly inorganic, fields, notably the texts by Z. L. Wang (Plenum Press, 1995), J. M. Cowley (Oxford University Press, 1993) and J. C. H. Spence & J. M. Zuo (Plenum Press, 1992), in showing the extent to which traditional X-ray theoretical methods combined with low-dose high-resolution microscopy are currently being applied over a wide range of compounds.

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