

would give $R_2 = 0.50$ or 0.74 , which are not overwhelmingly smaller.

The situation is perhaps a little more favourable on starting from an entirely wrong structure, and moving the atoms so as to reduce R_2 – the Booth approach. With all atoms wrongly placed $\Sigma_{cw} = \Sigma_o$. If some atoms (one atom and its symmetry-related equivalents, or perhaps a structural fragment and its equivalents) are now moved to their correct positions,

$$\Sigma_{cw} = \Sigma_o - \Sigma_{cc}, \quad (5)$$

$$T_{cw} = T_o - T_{cc}, \quad (6)$$

and (2) becomes

$$R_2 = 2 - \frac{2\Sigma_o^2}{(k+1)\Sigma_o^2 - QT_o} - 2 \frac{k\Sigma_{cc}^2 - QT_{cc}}{(k+1)\Sigma_o^2 - QT_o}. \quad (7)$$

This reduces to the expected values (Wilson, 1974) for no atoms correct and for all atoms correct. The first two terms are constants, and the third term represents a genuine reduction in R_2 as the atoms reach their correct positions.

One can compare the Booth and Lenstra approaches qualitatively by writing approximate equations for the case of equal atoms and terms in T neglected. If the total number of atoms is N , and the number of correctly placed atoms is n , the Lenstra approach gives

$$R_2 = 1 - 2n/(k+1)N - (k-1)n^2/(k+1)N^2, \quad (8)$$

(equation 2), whereas the Booth approach gives

$$R_2 = 2k/(k+1) - 2kn^2/(k+1)N^2 \quad (9)$$

(equation 7). If the atoms in the Lenstra approach are all wrongly placed,

$$R_2 = 1 - 2n/(k+1)N + n^2/N^2. \quad (10)$$

The discriminatory part of the reduction in R_2 is of the second order in n/N in both approaches, but in the Booth approach it is the only reduction, not confused by the larger first-order reduction that occurs in the Lenstra approach, whether the atoms are correctly placed or not. It would seem, therefore, that the Booth approach has a somewhat higher chance of being successful.

References

- BERTAUT, E. F. (1955). *Acta Cryst.* **8**, 537–543.
 BOOTH, A. D. (1947). *Nature, Lond.* **160**, 196.
 BOOTH, A. D. (1949). *Proc. Roy. Soc. A* **197**, 336–355.
 FOSTER, F. & HARGREAVES, A. (1963). *Acta Cryst.* **16**, 1124–1139.
 LENSTRA, A. T. H. (1974). *Acta Cryst.* **A30**, 363–369.
 LIPSON, H. & COCHRAN, W. (1953). *The Determination of Crystal Structures*. London: Bell.
 PARTHASARATHY, S. & PARTHASARATHI, V. (1972). *Acta Cryst.* **A28**, 426–432.
 QURASHI, M. M. (1949). *Acta Cryst.* **2**, 404–409.
 WILSON, A. J. C. (1942). *Nature, Lond.* **150**, 151–152.
 WILSON, A. J. C. (1969). *Acta Cryst.* **B25**, 1288–1293.
 WILSON, A. J. C. (1974). *Acta Cryst.* **A30**, 836–838.
 WILSON, A. J. C. (1976). *Acta Cryst.* **A32**, 53–56.

International Union of Crystallography

International Tables for X-ray Crystallography

Volume I (*Symmetry Tables*) of *International Tables for X-ray Crystallography* has been reprinted and is now available. The Executive Committee had previously decided not to reprint it because the first volume of the new series, on direct space, was expected to be published early in 1977. However, its publication has been delayed and it was felt that a reprint of the present Volume I would be necessary in the meantime.

Because of increases in printing costs it has been necessary to raise the price of Volume I to £15.00 and, because of the steady drop in the value of sterling with respect to other currencies, it has also been necessary to revise the sterling prices of the other volumes. Volume II (*Mathematical Tables*) and Volume III (*Physical and Chemical Tables*) now cost £11.50 each, whilst Volume IV (*Revised and Supplementary Tables for Volumes II and III*) costs £14.00. Copies may be obtained at the special reduced prices of £10.00 for Volume I, £6.00 for Volumes II or III and £9.00 for Volume IV by *bona fide* crystallographers, who must give an undertaking when purchasing that the volume is for their personal use only. Orders may be placed direct with the publishers, The Kynoch Press, Witton, Birmingham B6 7BA, England, or with Polycrystal Book Service, PO Box 11567, Pittsburgh, Pa. 15238, USA, from whom prospectuses may also be obtained.

Commission on Crystallographic Apparatus Exhibition of Non-Commercial Equipment and Visual Aspects of Crystallography at the

Eleventh International Congress of Crystallography

During the Eleventh International Congress of Crystallography, to be held in Warsaw, 3–12 August 1978, the Union's Commission on Crystallographic Apparatus is sponsoring two exhibitions, one of non-commercial crystallographic equipment and the other on visual aspects of crystallography. Crystallographers are invited to participate actively by displaying devices, gadgets charts, striking and unusual photographs, etc.

Non-commercial equipment

Items of interest to those attending the Congress include new designs or unique modifications of: cameras and diffractometers, high- and low-temperature attachments, high- and low-pressure equipment, crystal-growing apparatus, miscellaneous gadgets which are not intended for commercial exploitation.

The Committee will be able to furnish exhibition space and standard electric outlets (220 V, 50 Hz, 10 A single phase). Items requiring water or high power can be exhibited but not operated.