

more than 30% even for $|E| > 2.0$. It may be concluded that even though (1) can give good sign estimates for a crystal with weak anomalous scatterers or light atoms only, the

useful approximate methods, e.g. Harker construction, cannot be used for the solution of the phase problem, because the amplitude differences would be too small to measure accurately.

For the small structures it is seen that the sign distributions shown in Table 1 are only moderately influenced by the halogens. If the I, Br or Cl atom is replaced by F or even by H, the sign estimates for these light-atom crystals are still good; however, intensity differences of Friedel pairs may be too small to be measured accurately and no atom can be considered as a satisfactory anomalous scatterer for phasing by Harker construction.

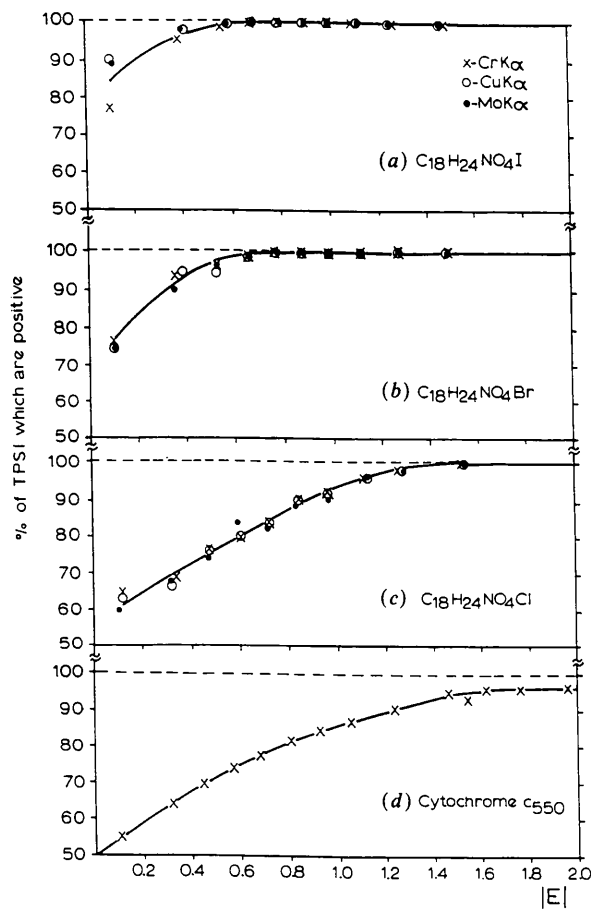


Fig. 1. Percentage of the TPSI's which are positive as a function of $|E|$.

Concluding remarks

The expectation of Hauptman's theory for estimating the TPSI signs, employing the chemical composition only, has been compared with the computational results for a series of crystals and wavelengths. The entries in Table 1 and the curves in Fig. 1 show that: (i) there exists a strong tendency towards positive signs of TPSI, and, as expected, the larger the $|E|$ values the more reliable are the sign estimates; (ii) the distributions are essentially independent of wavelength for the three small structures; (iii) the sign distributions do not strongly depend on the major anomalous scatterer I, Br, Cl etc. A detailed paper on the application of this procedure to protein structures is in preparation.

This work was supported by the Chinese NSF.

References

- CASCARANO, G. & GIACOVAZZO, C. (1984). *Acta Cryst.* **A40**, 305-306.
 FORTIER, S., FRASER, M. E. & MOORE, N. J. (1986). *Acta Cryst.* **A42**, 149-156.
 GIACOVAZZO, C. (1983). *Acta Cryst.* **A39**, 585-592.
 GUO, D. Y. & HAUPTMAN, H. (1989). *Chin. Sci. Bull.* **34**, 137-141.
 HAUPTMAN, H. (1982). *Acta Cryst.* **A38**, 632-641.
 SHEN, M. & RUBLE, J. R. (1975). *Acta Cryst.* **B31**, 2706-2709.
 TIMKOVICH, R. & DICKERSON, R. E. (1976). *J. Biol. Chem.* **251**, 4033-4046.

Books Received

The following books have been received by the Editor. Brief and generally uncritical notices are given of works of marginal crystallographic interest; occasionally a book of fundamental interest is included under this heading because of difficulty in finding a suitable reviewer without great delay.

Acta Cryst. (1990). **A46**, 944

Biominalisation: chemical and biochemical perspectives. Edited by S. MANN, J. WEBB and R. J. P. WILLIAMS.

Pp. xiv + 541. Weinheim, New York: VGH Verlag, 1988. Price DM 274.00. A review of this book, by S. K. Chapman, has been published in the August 1990 issue of *Acta Crystallographica*, Section B, pages 575-576.

A revolution in biotechnology. Edited by JEAN L. MARX. Pp. 227. Cambridge University Press, 1989. Price £25.00, US \$44.50. A review of this book, by J. R. Helliwell, has been published in the August 1990 issue of *Acta Crystallographica*, Section B, page 576.