LETTERS TO THE EDITOR

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X-ray anomalous-dispersion data and biomacromolecular crystal structure reports

BY R. SRINIVASAN

Department of Crystallography and Biophysics, University of Madras, Madras-25, India

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X-ray anomalous scattering has been playing an ever increasing role in structural crystallography during the last four decades (Bijvoet, Burgers & Hägg, 1969; Srinivasan, 1972; Ramaseshan & Abrahams, 1975). The need for careful preservation of intensity (or amplitude) data on *Bijvoet pairs* that may be collected through diffractometry or any other mode of collection and for the data to be available in suitable form in order to be able to extract $F(H)$ and $F(\bar{H})$ values individually was emphasized earlier (Srinivasan, 1970). With the advent of synchrotron radiation this aspect assumes, all the more, high importance since λ tunability enables larger values of the dispersion components f' and f'' to be realized (*e.g.* see Templeton & Templeton, 1990). The type of 'core structure' determination demonstrated for tartaric acid (Srinivasan & Chacko, 1967; Srinivasan, 1976) has been found useful for the location of S atoms in the case of a protein structure (Sheriff & Hendrickson, 1987), by first locating a heavier anomalous scatter (Fe). This also points to the possibility of a reductionistic approach to phase solution in protein crystallography since, from Bijvoet differences, the smaller set of anomalous scatters can be located, which can possibly act as the nucleus for enlarging the structure to the full protein. The anisotropic behaviour of dispersion effects (Templeton & Templeton, 1990) is also representable by this approach.

Apart from the above essentially unique solution to the phase problem by the single-wavelength anomalous-dispersion (SWAD) technique (Srinivasan & Chacko, 1970; Karle, 1985), extension to two wavelengths (Srinivasan & Chacko, 1970) and multiple-wavelength anomalous-dispersion (MAD) techniques (*e.g.* see Fourme & Hendrickson, 1990) hold promise in macromolecular crystallography. Study of finer variation in λ-dependent

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core-structure behaviour also becomes possible for macromolecules. In the context of macromolecular structural reports, I feel constrained to repeat my earlier observation with regard to small-molecule structures (Srinivasan, 1970) and to re-emphasize the need for special attention to be paid to data collection (whether or not Bijvoet difference data are used), preservation of $F(H)$, $F(\bar{H})$ data and reporting the same. The attention of the IUCr Commission on Macromolecules is invited to this aspect.

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