associated with a given set of phases $\{\varphi\}$; then, if we change $\varphi_{\mathbf{h}}$ to $\tilde{\varphi}_{\mathbf{h}} = \varphi_{\mathbf{h}} + \pi$ for an arbitrary number of reflections, the corresponding optimal $\nu_{\mathbf{h}}(\tilde{\varphi})$ will simply be $-\nu_{\mathbf{h}}(\varphi)$; this is clear from (1), which also tells us that the map $m(\mathbf{r})$ is unchanged, in contradiction with the results presented in SPSG. Thus, either the optimization problem described in SPSG is correct and there is a unique solution, independent of any sign combination, or there are several solutions and the algorithm of SPSG is not correct. In this latter case, the true Hessian matrix *cannot* be positive definite and *cannot* be given by equations (7) to (10) in SPSG (we recall that a function whose matrix of second derivatives, *i.e.* the Hessian, is everywhere positive semidefinite has at most one minimum). In any case, the procedure is not appropriate to explore the domain of possible phases of the structure factors.

The *ab initio* problem in crystallography is a very difficult one indeed. The Lagrangian approach by maximum entropy, already developed by Navaza (1985, 1986), has been given a firm mathematical basis: both for the statistical aspect (Gamboa, 1989; Dacunha-Castelle & Gamboa, 1990) and for its formulation as an optimization problem (Borwein & Lewis, 1991; Decarreau, Hilhorst, Lemaréchal & Navaza, 1991). To find a point where the gradient of the entropy with respect to the phases vanishes is a relatively easy task (given the available software); but the real numerical issue is to have a local maximum, *i.e.* a negative definite Hessian – quite another problem! All our experiments have unambiguously indicated that the entropy of a map is not a reliable figure of merit.

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LETTERS TO THE EDITOR

Contributions of a scientific nature intended for this section should be submitted to the Editor or any of the Co-Editors of Acta Crystallographica *or* Journal of Applied Crystallography.

Acta Cryst. (1991). A**47**, 632–633

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

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(*Received* 4 *February* 1991; *accepted* 30 *April* 1991)

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

0108-7673/91/050632-02$03.00

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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