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A comment on Hawthorne's paper *Refinement of merohedrally twinned crystals.*

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Comment is made on the paper by Hawthorne, F. C. [*Acta Cryst.* (1974). A30, 603–604].

In the procedure outlined by Hawthorne (1974) for the refinement of crystal structure by the least-squares method with intensities from merohedrally twinned crystals, the structure factors calculated for the two crystals in the twin are summed. By introducing linear constraints in the least-squares refinement program, as stated by the author, the newly generated parameters are used to calculate additional structure-factor components to be added to the original. But, instead, it is the intensities calculated for the two crystals in the twin which have to be added to get the total intensity. The program has to be rewritten to minimize $w\{I_o-(I_1+I_2)\}^2$ where I_o is the observed intensity, I_1 and I_2 are the calculated intensities due to the two crystals in the twin and w is the weight assigned for each observed intensity.

Reference

HAWTHORNE, F. C. (1974). *Acta Cryst.* A30, 603–604.

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Efficiency in Fourier phase refinement for protein crystal structures.

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Fourier phase refinement for macromolecular crystal structures can be accomplished using electron density maps sampled at intervals of half the minimum interplanar spacing for which diffraction data have been measured in that direction. Order-of-magnitude economy in computation is thus gained as compared to use of customary sampling rates.

Fourier phase refinement is a much discussed method for improvement of the crystallographic description of large biological molecules [see, *e.g.*, Barrett & Zwick (1971) and references cited therein]. Use of this method certainly will become more widespread as the real cost of computing decreases and computer programs based on Fast Fourier Transform algorithims become freely available. Notwithstanding the present speed and efficiency of Fourier inversion, repetitive calculations for crystals with large asymmetric units still require a most substantial investment of computational resources. In the interest of further economy we have examined the proposition that the sampling criterion of Lipson & Cochran (1966) must be satisfied in Fourier phase-refinement calculations, as implied by Barrett & Zwick (1971).

The conceptual cornerstone of these refinement calculations is the idea that a mediocre electron density map (*i.e.* a map based on experimental structure amplitudes and estimated phases) can be modified in a reasonable way to provide a density function rather more similar to the true density function than was the original (Hoppe & Gassmann, 1968). This being so, it is a simple matter to transform the modified density function and obtain improved phases. This concept was first presented by Sayre (1952) who gave the relationships

$$\varrho(\mathbf{r}) \sim \varrho^2(\mathbf{r}), \tag{1a}$$

and consequently,

$$F_{\mathbf{h}} = \frac{1}{V}\theta_{\mathbf{h}} \sum_{\mathbf{K}} F_{\mathbf{k}} F_{\mathbf{h}-\mathbf{k}}, \tag{1b}$$

where V is the unit cell volume and θ is a shape function. The development of these equations has been directed principally toward use of the latter in *ab initio* estimation of phases for crystal structures of moderate complexity. In fact, (1*b*) and similar equations have been so successful in application that many crystallographers have come to think of (1*b*) as a fundamental relationship among structure

Table 1. *Figures of merit and convergence during phase refinement*

All numbers are given in pairs; the upper is for case I, the lower for case II as described in the text.

		Iteration				
		0	1	2	3	4
Average change in phase angle (°)*	I	—	32 (37)	17 (20)	6 (8)	2 (4)
	II	—	32 (37)	16 (19)	5 (8)	2 (4)
R†	I	—	0·28	0·21	0·19	0·19
	II	—	0·26	0·21	0·21	0·22
Average error in phase angle (°)*	I	46 (46)	26 (32)	17 (24)	15 (22)	15 (22)
	II	46 (46)	24 (29)	16 (23)	16 (23)	17 (24)

* Modulus-weighted averages are given; the corresponding unweighted averages are in parentheses.
† R is calculated from $R=\sum||F_{\text{exp}}|-|F_{\text{calc}}||/\sum|F_{\text{exp}}|$.