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Comments on the short communication, *A statistical evaluation of absorption* by C. Katayama, N. Sakabe and K. Sakabe.

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In a recent paper by Katayama, Sakabe & Sakabe [*Acta Cryst.* (1972), A28, 293] some principles of an empirical absorption correction method are described. These have been published previously [Kopfmann & Huber (1968). *Acta Cryst.* A24, 348].

Katayama, Sakabe & Sakabe (1972), in describing their method of absorption correction, referred to the paper of North, Phillips & Mathews (1968). In the same issue of *Acta Crystallographica* we have proposed a general method of empirical absorption correction by X-ray intensity measurements. Our paper stresses the application to crystals with arbitrary shapes and the use of multiple measurements of the same reflexion and equivalent reflexions for the determination of absorption. General formulae as well as special algorithms for the numerical evaluation of the absorption correction were given. The application of the method to proteins has been pointed out and experimental results have been published in another paper (Huber & Kopfmann, 1969).

In a recent short communication (Katayama, Sakabe & Sakabe, 1972) some principles of this method are described again and the general algorithm in our first paper [equation (10), page 351 of Kopfmann & Huber, 1968] is presented as a special case [equation (3) in the short communication]. Furthermore the least-squares evaluation of these authors is restricted to equivalent reflexions, limited in number by the space group, whereas in our method, as many observations of the same reflexion as necessary may be used by a rotation about the reciprocal-lattice vector.

In our opinion no new detail has been given in the short communication of these authors.

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The usefulness of the generalized tangent formula.

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The generalized form of the tangent formula [Tsai, C-C. & Collins, D. M. (1972). *Acta Cryst.* B28, 1601] cannot work except for the trivial case where the generalized form equals the ordinary tangent formula. The T'_{21} formula is in contradiction with the Harker–Kasper inequality for $\bar{1}$.

Recently Tsai & Collins (1972) described a generalized form of the tangent formula:

$$\tan(r\varphi_H) \simeq \frac{\sum_K |E_K|^p |E_{\frac{r}{q}H-\frac{p}{q}K}|^q \sin\left(p\varphi_K + q\varphi_{\frac{r}{q}H-\frac{p}{q}K}\right)}{\sum_K |E_K|^p |E_{\frac{r}{q}H-\frac{p}{q}K}|^q \cos\left(p\varphi_K + q\varphi_{\frac{r}{q}H-\frac{q}{q}K}\right)}. \quad (1)$$

They use in the phase-determining procedure the following special cases of (1):

$$\tan(\varphi_H) \simeq T'_{11} = \frac{\sum_K |E_K E_{H-K}| \sin(\varphi_K + \varphi_{H-K})}{\sum_K |E_K E_{H-K}| \cos(\varphi_K + \varphi_{H-K})} \quad (2)$$

the well known tangent formula and

$$\tan(\varphi_H) \simeq T'_{22} = \frac{\sum_K |E_K|^2 |E_{H-2K}| \sin(2\varphi_K + \varphi_{H-2K})}{\sum_K |E_K|^2 |E_{H-2K}| \cos(2\varphi_k + \varphi_{H-2K})}. \quad (3)$$

Whereas the reliability of a single term of (2) is a function of $|E_H E_K E_{H-K}|$, the reliability of a single term of (3) is a function of $|E_H E_K^2 E_{H-2K}|$.

The purpose of this paper is to show that in centrosymmetric structures (3) does not work. In our opinion the only useful form of (1) is that with $p=q=r=1$, the ordinary tangent formula (2).

For centrosymmetric structures (3) reduces to

$$\cos(\varphi_H) = \frac{\sum_K |E_K|^2 |E_{H-2K}| \cos(2\varphi_K + \varphi_{H-2K})}{\sum_K |E_K|^2 |E_{H-2K}|}. \quad (4)$$

Because $\varphi_K = 0$ or π, equation (4) is equal to

$$\cos(\varphi_H) = \frac{\sum_K |E_K|^2 |E_{H-2K}| \cos\varphi_{H-2K}}{\sum_K |E_K|^2 |E_{H-2K}|}. \quad (5)$$

Equation (5) states that the signs $S(H)$ of H and $S(H-2K)$ of $H-2K$ are equal if the normalized structure factors