fragments were isolated, were prepared by Dr C. J. Raub. One of the two crystal spheres was ground by Miss H. A. Plettinger. The least-square refinement was carried out on the IBM 704 computer of the Argonne National Laboratory. The work was in part supported by the Advanced Research Projects Agency.

The investigation reported in this paper was begun during a visit to the University of California at San Diego. The writer thanks Prof. B. T. Matthias and other La Jolla friends for valuable discussions in a hospitable milieu.

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## Short Communications

*Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible. Publication will be quicker if the contributions are without illustrations.*

*Acta Cryst.* (1963). **16**, 1255

### The crystal structure of KI.Hg(CN)$_2$. A correction.

By F. H. KRUSE, *Los Alamos Scientific Laboratory, Los Alamos, New Mexico, U.S.A.*

(*Received* 21 *March* 1963)

The paper of the above title (Kruse, 1963) contains an error in Table 4 — *Final observed and calculated structure factors for* KI.Hg(CN)$_2$.

The $F_o$ values for reflections 001, 003, 005, and 009 should be marked with a minus sign denoting 'less than' for these unobserved values, thus making the data table compatible with the space group, *Cmcm*.

#### Reference

KRUSE, F. H. (1963). *Acta Cryst.* **16**, 105.

*Acta Cryst.* (1963). **16**, 1255

### Treatment of anomalous dispersion in X-ray diffraction data.

By A. L. PATTERSON, *The Institute for Cancer Research, Fox Chase, Philadelphia* 11, *Pennsylvania, U.S.A.*

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The purpose of this note is to reemphasize and to amplify the remarks made by Templeton (1955) concerning the importance of the correction of X-ray data for anomalous dispersion effects in the refinement of crystal structures. We are not concerned here with the important uses of such data in the initial approach to the solution of the phase problem.

First, let us assume that there is only one element in the crystal which shows appreciable dispersive effects. This element may be located in one or more sets of general or special positions and is assumed to have structure factor components $A_d = f_d H_d$ and $B_d = f_d K_d$ where $f_d$ is the non-dispersive part of the scattering factor for the dispersive atom at rest and the geometrical components $H_d$ and $K_d$ are assumed to contain isotropic or anisotropic temperature factors appropriate for the thermal motion of the atoms of the dispersive element in the crystal. The structure factor components for the non-dispersive part of the crystal are taken as $A_n$ and $B_n$. We define $F_+$ as the structure factor for the plane $hkl$ for which $A_n, B_n, A_d, B_d$ are calculated. Then $F_-$ is that for the plane $\bar{h}\bar{k}\bar{l}$ the inverse of the first. The structure factors for these two planes may then be written in the well known form (*cf.* James, 1948)

$$F_\pm = A_n + i\sigma B_n + (H_d + i\sigma K_d)(f_d + \Delta f'_d + i\Delta f''_d)\,, \quad (1)$$

in which $\sigma = +1$ corresponds to $F_+$, $\sigma = -1$ corresponds to $F_-$, and $\Delta f'_d$ and $\Delta f''_d$ are the real and imaginary components of the dispersive effect for the given atom. The result (1) may then be rewritten in the forms

$$\begin{aligned} F_\pm &= A_n + i\sigma B_n + (A_d + i\sigma B_d)(1 + \delta_1 + i\delta_2) \\ &= (A + \delta_1 A_d - \sigma\delta_2 B_d) + i\sigma(B + \delta_1 B_d + \sigma\delta_2 A_d)\,, \end{aligned} \quad (2)$$

where $A$ and $B$ are the non-dispersive structure factor components for the whole structure, and

$$\delta_1 = \Delta f'_d / f_d\,; \quad (2a)$$

$$\delta_2 = \Delta f''_d / f_d\,. \quad (2b)$$

We now calculate

$$|F_\pm|^2 = A^2 + B^2 + (\delta_1^2 + \delta_2^2)(A_d^2 + B_d^2) + 2\delta_1(AA_d + BB_d) - 2\sigma\delta_2(AB_d - BA_d) \quad (3)$$

and define the quantities $S$ and $D$ as

$$S = \tfrac{1}{2}\{|F_+|^2 + |F_-|^2\} = A^2 + B^2 + 2\delta_1(AA_d + BB_d) + (\delta_1^2 + \delta_2^2)(A_d^2 + B_d^2) \quad (4a)$$

and

$$D = \tfrac{1}{2}\{|F_+|^2 - |F_-|^2\} = -2\delta_2(AB_d - BA_d)\,. \quad (4b)$$

One could of course make use of formula (3) to calculate