This equation is the acdf of Vainstein (1966) and is equivalent to his equation (152).

The aim of this note is to draw attention to the lack of definition of the  $\rho'_0$  in the acdf (equation 5). It will be clear that equation (4) does not define  $\rho'_0$ . From equation (1) the most logical choice of  $\rho'_0$  would appear to be

$$\varrho'_0 = \int_{-h}^{+h} \varrho_0 \mathrm{d}z = 2h\varrho_0 \tag{6}$$

but this still does not define  $\varrho'_0$ , since the value of h is not fixed. This lack of definition of  $\varrho'_0$  has, to our knowledge, not been recognized. Because of it, the usefulness of equation (5) is limited, and certainly the areas under the peaks of the acdf cannot be interpreted in terms of the numbers of neighbors as has been done in the literature (Chistyakov, 1964; Chistyakov & Vainshtein, 1963). That it is incorrect to do so follows from the fact that by varying  $\varrho'_0$  one can arbitrarily change the areas under the peaks. Putting it another way, since the acdf deals with the numbers of atoms in cylindrical shells of undefined height (2h), these numbers are not defined either. Moreover, the term 'neighbors' loses its meaning for atoms in a cylindrical shell: some of these atoms (those with small z) may be rather close to the reference atom p, whereas others (with large z) are quite far away from it.

For these reasons it is preferable to use equation (3), or  $2\pi a$  times equation (3), for acdf studies; unlike  $\varrho'(a)$  and  $\varrho'_0$ ,  $\Delta \varrho'(a)$  is a well defined quantity, not dependent upon the choice of h.

For the *molecular* cylindrical distribution function (mcdf) the same argument holds: here too, the areas under the peaks should not be correlated with the number of neighbors of a molecule, as done in the literature (*e.g.* Kosterin & Chistyakov, 1969). There also appear to be other serious problems connected with the mcdf. These require a detailed analysis of the mcdf and its derivation, and will be discussed elsewhere (De Vries, 1972).

## References

- ALEXANDER, L. E. & MICHALIK, E. R. (1959). Acta Cryst. 12, 105.
- CHISTYAKOV, I. G. (1964). J. Struct. Chem. USSR, 5, 507.
- CHISTYAKOV, I. G. & CHAIKOVSKII, V. M. (1967). Sov. Phys. Crystallogr. 12, 770.
- CHISTYAKOV, I. G. & CHAIKOVSKII, V. M. (1969). Mol. Cryst. Liquid Cryst. 7, 269.
- CHISTYAKOV, I. G. & VAINSHTEIN, B. K. (1963). Sov. Phys. Crystallogr. 8, 458.
- DELORD, P. (1969). J. Phys. Radium, 30, C4, p. 14.
- DELORD, P. & FALGUEIRETTES, J. (1968a). C. R. Acad. Sci. Paris, C267, 1437.
- DELORD, P. & FALGUEIRETTES, J. (1968b). C. R. Acad. Sci. Paris, C267, 1528.
- DELORD, P. & MALET, G. (1970). C. R. Acad. Sci. Paris. B270, 1107.
- DE VRIES, A. (1972). J. Chem. Phys. 56, 4489.
- GUSAKOVA, L. A. & CHISTYAKOV, I. G. (1968). Sov. Phys. Crystallogr. 13, 452.
- JAMES, R. W. (1958). The Optical Principals of the Diffraction of X-rays, p. 477. London: Bell.
- Kosterin, E. A. & Chistyakov, I. G. (1968). Sov. Phys. Crystallogr. 13, 229.
- Kosterin, E. A. & Chistyakov, I. G. (1969). Sov. Phys. Crystallogr. 14, 252.
- MARGENAU, H. & MURPHY, G. M. (1950). The Mathematics of Physics and Chemistry, p. 251. New York: Van Nostrand.
- OSTER, G. & RILEY, D. P. (1952). Acta Cryst. 5, 272.
- VAINSHTEIN, B. K. (1966). Diffraction of X-rays by Chain Molecules, p. 251. Amsterdam: Elsevier.
- VAINSHTEIN, B. K., CHISTYAKOV, I. G., KOSTERIN, E. A. & CHAIKOVSKII, V. M. (1967). Sov. Phys. Dokl. 12, 405.
- VAINSHTEIN, B. K., CHISTYAKOV, I. G., KOSTERIN, E. A. & CHAIKOVSKII, V. M. (1969). Mol. Cryst. Liquid Cryst. 8, 457.

Acta Cryst. (1972). A28, 660

Comments on the paper, The determination of cyclicity hexagonality and other properties of polytypes by Dornberger-Schiff, Schmittler and Farkas-Jahnke: Erratum. By J. KAKINOKI, E. KODERA and T. AIKAMI, Department of Physics, Faculty of Science, Osaka City University, Sugimoto-cho, Sumiyoshi-ku, Osaka, Japan

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Corrections are given to Acta Cryst. (1972). A28, 292.

(1) Page 292, column 2, line 14: '  $\$  and  $\$  ' should be

tion should be performed over s not from 2 but from 0 to t-1.

## read as ' $\mathcal{S}$ and $\mathcal{S}$ '.

(2) Page 293, column 2, the first term in the larger parentheses in expression of  $D_m^*$  for m=3r-1: The summa-

KAKINOKI, J., KODERA, E. & AIKAMI, T. (1972). Acta Cryst. A 28, 292.

References