

polarization factors (Waser, 1951), but not corrected for absorption, and a least-squares refinement was computed on Maniac II. The scale factor, two isotropic temperature factors and the two  $y$  parameters were simultaneously refined. All terms of the normal equations were used. The Thomas-Fermi form-factor was used for Pu and the form-factor computed by Viervoll & Øgrim (1949) was used for Ni. Ten electrons were subtracted from the Pu form factor as an approximate correction for anomalous dispersion. The results of the refinement are

$$y_{\text{Pu}} = 0.1421 \pm 0.0009, \quad y_{\text{Ni}} = 0.4221 \pm 0.0034, \\ B_{\text{Pu}} = 1.38 \pm 0.21, \quad B_{\text{Ni}} = 2.43 \pm 0.81.$$

The calculated and observed  $0kl$  structure factors, for which  $R = 10.9\%$ , are given in Table 1.

Each atom has seven neighbors of the opposite kind, four at 2.85, two at 2.88 and one at 2.86 Å. In addition, the Ni atom has two Ni neighbors at 2.64 Å and the

Pu has eight Pu neighbors, two at 3.54 and six at 3.59 Å. The estimated standard deviations are 0.02 Å for Pu-Pu, 0.04 Å for Pu-Ni and 0.05 Å for Ni-Ni distances.

We are indebted to V. O. Struebing and E. M. Cramer, of this Laboratory, for preparing and heat treating the alloy.

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*Acta Cryst.* (1959). **12**, 943

**A reply to some comments by Karle and Hauptman.** By A. KLUG, *Birkbeck College Crystallography Laboratory, University of London, 21 Torrington Square, London, W. C. 1, England*

(Received 12 June 1959)

In a recent paper Karle & Hauptman (1959) comment, in a lengthy footnote, on a paper of mine (Klug, 1958) on the phase problem. They state that in a previous paper of theirs (Karle & Hauptman, 1956) they had already derived 'measures of statistical significance based on the appropriate variances' of individual terms in phase-determining formulae. I did not refer to this paper earlier since the relevant discussion in it on variances is concerned with two points, both of which had already been adequately dealt with in earlier papers by other workers, which I did cite. The first point, on the degree of validity of a formula according as the atoms in the cell are equal or not, has been discussed by Cochran (1954) and Cochran & Woolfson (1955), while the second, on the weighting of the terms in a formula by their variances, had first been discussed by Bullough & Cruickshank (1955). In any case it is misleading to claim that the discussion in Karle & Hauptman's (1956) paper yields 'measures of statistical significance' that throw any critical light on the whole problem. No explicit mention is made there of the dependence of the variances and hence of the reliability of the formulae on the number of atoms in the unit cell, which, together with the finite amount of data, sets the principal limitation to the use of statistical or algebraic methods. Nor were the calculations made to a high enough order of accuracy to show how the *variance* of the estimate of the sign of a structure factor depends on the magnitudes of the  $E$ 's involved in the sign relation being studied (cf. expressions [3.20], [3.30], and [3.35] of my paper, and particularly [5.14] and the discussion following it). It is therefore not at all possible to study from Karle & Hauptman's calculations the effect of unusually large  $E$  values, on which the success of the formulae is expected to rest. Their newest approach (1959) suffers from the same defects so that it is not at all clear from it under what conditions the formulae given would be valid in practice.

These points, and others, were considered in my paper, in which measures of significance were given to phase-determining relations by introducing the concept of the order of a relation. My conclusion that only relations of the lowest order could be expected to be generally useful has been recently confirmed by Cochran (1958).

However, as Karle & Hauptman state, the most convincing test of any phase-determining theory is in its practical application to the solution of crystal structures. In view of the criticisms that have been made of their claim to have devised a *routine* procedure for solving the phase problem, valid whatever the number of atoms in the unit cell, it is to be hoped that failures, as well as successes, of the method will be recorded. Furthermore it would be generally very helpful to continue to assess (cf. Karle *et al.*, 1957), in the case of a successful application of the method to a structure of some complexity, which of the formulae played a key role in the solution, and also, if possible, to discuss the relation of these to other methods for solving crystal structures (cf. Wright (1958)).

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