

analyses have utilized the experimental data of GW. In the present study, the four parameters in the Dawson functions were determined from the present experimental data. The exponent  $\alpha$  of the radial distribution functions in (4) was found to be  $2 \cdot 10 (26) \text{ \AA}^{-2}$ . This value is almost the same as that assumed by Dawson as shown in Table 2. However, the values of the parameters  $K_{22}$  and  $L_{22}$  which were obtained are slightly different from those of Dawson. One can calculate the deformation charge density using these parameters. The maximum deformation density at the midpoint between the nearest-neighbour atoms is  $0 \cdot 44 (17) \text{ e\AA}^{-3}$ , which is smaller than Dawson's value of  $0 \cdot 63_5 \text{ e\AA}^{-3}$  as shown in Fig. 4.

In order to study the thermal vibration, the GW data have been recalculated for several charge density models (McConnell & Sanger, 1970; Stewart, 1973*a*; Price & Maslen, 1978). The  $B$  values obtained in the recalculations range from  $0 \cdot 14$  to  $0 \cdot 22 \text{ \AA}^2$  depending on the models used. On the other hand, the neutron diffraction studies have concluded that the values lie between  $0 \cdot 14$  and  $0 \cdot 17 \text{ \AA}^2$ . The present value of  $0 \cdot 142 (9) \text{ \AA}^2$  is in good agreement with the value calculated from the phonon dispersion curves measured by inelastic neutron scattering,  $0 \cdot 149$ – $0 \cdot 150 \text{ \AA}^2$  (Stewart, 1973*b*), and also with that from neutron diffraction of the powdered sample,  $0 \cdot 14$ – $0 \cdot 17 \text{ \AA}^2$  (Price, Maslen & Moore, 1978).

Synthetic diamond crystals were used as the specimens and these contained grown-in dislocations to a certain extent as shown in Fig. 1. The *Pendellösung* beats were measured only in the defect-free regions. However, it is inevitable that there are some effects

resulting from the strain field around the dislocations near the region used. Nevertheless, the effects are thought to be small, because the values of the structure factors obtained differ only slightly from each other in the different regions.

The authors are greatly indebted to Messrs S. Yazu and K. Tsuji of Sumitomo Electric Industries, Ltd, Japan for kindly supplying parallel-sided synthetic diamond wafers. They also acknowledge the partial support of this work by the Grant-in-Aid for Scientific Research from the Ministry of Education, Science and Culture of Japan (TT, 62460224 and 01580049).

#### References

- CROMER, D. T. & LIBERMAN, D. (1970). *J. Chem. Phys.* **53**, 1891–1898.  
 CROMER, D. T. & WABER, J. T. (1974). *International Tables for X-ray Crystallography*. Vol. IV. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)  
 DAWSON, B. (1967). *Proc. R. Soc. London Ser. A*, **298**, 264–288.  
 GÖTTLICHER, S. & WÖLFEL, E. (1959). *Z. Elektrochem.* **63**, 891–901.  
 KATO, N. (1968). *J. Appl. Phys.* **39**, 2225–2237.  
 KOBAYASHI, K., TAKAMA, T., TOHNO, S. & SATO, S. (1988). *Jpn. J. Appl. Phys.* **27**, 1793–1797.  
 LANG, A. R. & MAI, Z.-H. (1979). *Proc. R. Soc. London Ser. A*, **368**, 313–329.  
 MCCONNELL, J. F. & SANGER, P. L. (1970). *Acta Cryst.* **A26**, 83–93.  
 PRICE, P. F. & MASLEN, E. N. (1978). *Acta Cryst.* **A34**, 173–183.  
 PRICE, P. F., MASLEN, E. N. & MOORE, F. H. (1978). *Acta Cryst.* **A34**, 171–172.  
 RENNINGER, M. (1955). *Acta Cryst.* **8**, 606–610.  
 STEWART, R. F. (1973*a*). *J. Chem. Phys.* **58**, 4430–4438.  
 STEWART, R. F. (1973*b*). *Acta Cryst.* **A29**, 602–605.  
 TAKAMA, T. & SATO, S. (1988). *Aust. J. Phys.* **41**, 433–448.

*Acta Cryst.* (1990). **A46**, 517–520

## The Use of Structural Information in Phase Determination

BY E. A. KLOP, H. KRABBENDAM AND J. KROON

*Laboratorium voor Kristal- en Structuurchemie, Rijksuniversiteit, Padualaan 8, 3584 CH Utrecht, The Netherlands*

(Received 23 June 1989; accepted 31 January 1990)

### Abstract

The procedure adopted by Heinerman [*Acta Cryst.* (1977). **A33**, 100–106] to incorporate structural information in phase determination is combined with that of Giacovazzo [*Acta Cryst.* (1983). **A39**, 685–692]. The resulting joint probability distribution of three structure factors is a generalization of the corresponding distributions of the previous authors. This distribution is used (i) to calculate the phase of a triple product given *a priori* structural information, (ii) to

resolve the sign ambiguity in single isomorphous replacement if the replacement structure is known. The latter application for the incorporation of partial structure information is more general than that proposed by Fan Hai-fu & Gu Yuan-xin [*Acta Cryst.* (1985). **A41**, 280–284].

### Introduction

In the generalized Cochran formula proposed by Main (1976), four different types of *a priori* informa-

tion can be used, *viz* (a) randomly positioned atoms, (b) randomly positioned and randomly oriented atomic groups, (c) randomly positioned but correctly oriented atomic groups, (d) correctly positioned atomic groups (partial structure information). A mathematical derivation of this formula was given by Heinerman (1977). Case (d) was reconsidered by Giacovazzo (1983) and new mathematical formulae were obtained by a proper use of *a priori* information. Heinerman's (1977) approach can exploit different types of *a priori* information, but the allowed size of the group of atoms with known position is limited whereas Giacovazzo's (1983) approach does not exploit different types of *a priori* information but has no limit on the size of the group of atoms with known position.

Fan Hai-fu, Han Fu-son, Qian Jin-zi & Yao Jia-xing (1984) showed that the sign ambiguity that exists in single isomorphous replacement (SIR) can be resolved if the replacement structure is known. They based their treatment on the Cochran (1955) distribution. In an extension of their approach they incorporated partial structure information *via* Sim's distribution (Fan Hai-fu & Gu Yuan-xin, 1985). Subsequently, Hauptman's (1982) joint probability distribution for the SIR case was employed to obtain the sign probability if the replacement structure is known (Klop, Krabbendam & Kroon, 1987; Hao Quan & Fan Hai-fu, 1988).

In the first part of the paper we will combine the approach of Heinerman (1977) with that of Giacovazzo (1983) and calculate the probability distribution of a triplet-invariant phase given *a priori* information. In the second part the sign ambiguity in the SIR case will be resolved by exploiting *a priori* information using the results of the first part of the paper.

### Theory

In his derivation of the probability distribution of a triple product for space group  $P1$  given different types of structural information, Heinerman (1977) treated the position vector of the group of correctly placed atoms as a primitive random variable, thereby treating this group in the same way as the group of correctly oriented but randomly positioned atoms. In the approach adopted by Giacovazzo (1983), the position vectors of the randomly positioned atoms were regarded as the primitive random variables and the position vector of the group of correctly positioned atoms was not.

In the following we will start from Heinerman's (1977) approach and combine it with that of Giacovazzo (1983) by excluding the position vector of the group of correctly placed atoms from the set of primitive random variables. The notation of

Heinerman (1977) [ $H$ ] will be used throughout this paper. The structure factor  $F_{\mathbf{h}}$  is defined by

$$F_{\mathbf{h}} = \sum_{j=1}^p g_j(\mathbf{h}) \exp(2\pi i \mathbf{h} \cdot \mathbf{r}_j). \quad (1)$$

A subscript  $j$  labels an atom or group of atoms with scattering factor  $g_j(\mathbf{h})$  and position vector  $\mathbf{r}_j$ . Let  $j = p$  denote the group of atoms with known orientation and position. The factor  $g_p(\mathbf{h})$  is the known structure factor of this group and since the origin may be chosen anywhere in  $P1$ , we choose  $\mathbf{r}_p = \mathbf{0}$ . The normalized structure factor  $E_{\mathbf{h}}$  is defined by

$$E_{\mathbf{h}} = F_{\mathbf{h}} / \langle |F_{\mathbf{h}}|^2 \rangle_{\text{p.r.v.}}^{1/2}. \quad (2)$$

where the average in the denominator is taken over the primitive random variables (p.r.v.) of which there are three types corresponding to the first three categories of structural information referred to above:

- (a)  $1 \leq j \leq p_1$  atomic position vectors;
- (b)  $p_1 + 1 \leq j \leq p_2$  the position vectors and orientational parameters;
- (c)  $p_2 + 1 \leq j \leq p - 1$  the position vectors of the groups with known orientation (*i.e.* excluding the position vector of the group with known orientation and known position).

Note that (5)-(13) [ $H$ ] still apply.

We shall derive the joint probability distribution  $P(R_1, R_2, R_3, \varphi_1, \varphi_2, \varphi_3)$  of the magnitudes  $|E_{\mathbf{h}_1}|$ ,  $|E_{\mathbf{h}_2}|$ ,  $|E_{\mathbf{h}_3}|$  and the phases  $\varphi_{\mathbf{h}_1}$ ,  $\varphi_{\mathbf{h}_2}$ ,  $\varphi_{\mathbf{h}_3}$ , where  $\mathbf{h}_1 + \mathbf{h}_2 + \mathbf{h}_3 = \mathbf{0}$ , *via* its characteristic function  $Q(\rho_1, \rho_2, \rho_3, \theta_1, \theta_2, \theta_3)$ . The calculation of the characteristic function is given in Appendix I.\* The result replaces (15) [ $H$ ] and reads

$$\begin{aligned} & Q(\rho_1, \rho_2, \rho_3, \theta_1, \theta_2, \theta_3) \\ & \simeq \exp \left\{ -\frac{1}{4} i Q'_{123} \rho_1 \rho_2 \rho_3 \cos(\theta_1 + \theta_2 + \theta_3 - q'_{123}) \right. \\ & \quad \left. + \sum_{n=1}^3 [u_{pn} i \rho_n \cos(\beta_{pn} - \theta_n) - \frac{1}{4} (1 - u_{pn}^2) \rho_n^2] \right\}, \quad (3) \end{aligned}$$

where  $u_{pn} \equiv u_p(\mathbf{h}_n)$ ,  $\beta_{pn} \equiv \beta_p(\mathbf{h}_n)$  and  $Q'_{123} \exp q'_{123}$  is given by (16) [ $H$ ] with  $p$  in the third term replaced by  $p - 1$ . The Fourier transformation in Appendix IV [ $H$ ] is replaced by Fourier transformation of (3). The

\* Appendices I and II have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52660 (7 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

result replaces (21) [ $H$ ] and reads

$$\begin{aligned}
 P(R_1, R_2, R_3, \varphi_1, \varphi_2, \varphi_3) \\
 \approx (R_1 R_2 R_3 / \pi^3) [(1 - u_{p1}^2)(1 - u_{p2}^2)(1 - u_{p3}^2)]^{-1} \\
 \times \exp \left\{ \sum_{n=1}^3 -(1 - u_{pn}^2)^{-1} \right. \\
 \times [R_n^2 + u_{pn}^2 - 2R_n u_{pn} \cos(\varphi_n - \beta_{pn})] \\
 + 2Q'_{123} / [(1 - u_{p1}^2)(1 - u_{p2}^2)(1 - u_{p3}^2)] \\
 \times [R_1 R_2 R_3 \cos(\varphi_1 + \varphi_2 + \varphi_3 - q'_{123}) \\
 - u_{p1} R_2 R_3 \cos(\beta_{p1} + \varphi_2 + \varphi_3 - q'_{123}) \\
 - R_1 u_{p2} R_3 \cos(\varphi_1 + \beta_{p2} + \varphi_3 - q'_{123}) \\
 - R_1 R_2 u_{p3} \cos(\varphi_1 + \varphi_2 + \beta_{p3} - q'_{123}) \\
 + u_{p1} u_{p2} R_3 \cos(\beta_{p1} + \beta_{p2} + \varphi_3 - q'_{123}) \\
 + u_{p1} R_2 u_{p3} \cos(\beta_{p1} + \varphi_2 + \beta_{p3} - q'_{123}) \\
 + R_1 u_{p2} u_{p3} \cos(\varphi_1 + \beta_{p2} + \beta_{p3} - q'_{123}) \\
 \left. - u_{p1} u_{p2} u_{p3} \cos(\beta_{p1} + \beta_{p2} + \beta_{p3} - q'_{123}) \right\}. \quad (4)
 \end{aligned}$$

Now, consider the following special cases.

(i) If there is little partial structure information then  $u_{pn} \approx 0$  ( $n = 1, 3$ ) and (4) reduces to (21) [ $H$ ]. The latter equation is valid only for small  $u_p$ , *i.e.* for small partial structures, as was observed by Heinerman [ $H$ ], whereas (4) is valid for all  $u_p \neq 1$ .

(ii) For the limiting case that the whole structure is known  $Q'_{123} = 0$  and  $u_{pn} = 1$  ( $n = 1, 3$ ). Introduction of this into (3) followed by Fourier transformation gives a delta function centred on  $R_n = 1$  and  $\varphi_n = \beta_{pn}$  ( $n = 1, 3$ ).

(iii) If there is no other structural information than partial structure information (apart from the information provided by the atomic hypothesis, the basic source of structural information in direct methods) then  $Q'_{123} = c$ ,  $q'_{123} = 0$ ,  $(1 - u_{pn}^2) = b_n$ ,  $u_{pn} = R_{pn}$  ( $n = 1, 3$ ) with  $c$ ,  $b_n$  and  $R_{pn}$  defined by Giacovazzo (1983). The distribution defined in (19) of Giacovazzo (1983) employs partial structure information [*i.e.* type ( $d$ )] as the only source of structural information and turns out to be a special case of (4), after correcting the (probably clerical) error ( $-$  becomes  $+$ ) in the last line of (19).

Appendix II (deposited) contains the calculation of the conditional distribution  $P(\Phi | R_1, R_2, R_3)$  of the phase  $\Phi = \varphi_1 + \varphi_2 + \varphi_3$  given the magnitudes  $|E_{h_1}|$ ,  $|E_{h_2}|$  and  $|E_{h_3}|$  which is obtained from (4). If only terms up to third order in the  $u_{pi}$  are retained in (II.10) the result is the von Mises distribution

$$\begin{aligned}
 P(\Phi | R_1, R_2, R_3) \\
 \approx (1/L) \exp \{ 2Q'_{123} R_1 R_2 R_3 \cos(\Phi - q'_{123}) \\
 + 2u_{p1} u_{p2} u_{p3} R_1 R_2 R_3 \cos(\Phi - \Phi_p) \} \\
 = (1/L) \exp \{ 2Q_{123} R_1 R_2 R_3 \cos(\Phi - q_{123}) \}, \quad (5)
 \end{aligned}$$

where  $\Phi_p = \beta_{p1} + \beta_{p2} + \beta_{p3}$ ,  $L = 2\pi I_0(2Q_{123} R_1 R_2 R_3)$  and  $Q_{123}$  and  $q_{123}$  as defined by Heinerman, hence (5) is identical to (22) [ $H$ ]. Heinerman's derivation is based on a simpler joint probability distribution, valid only for small  $u_{pi}$ , from which his conditional distribution can be obtained without further approximations. Although our derivation is based on the joint probability distribution (4) which holds for any  $u_p \neq 1$ , approximations are necessary in the derivation of the conditional distribution so that the conditional distribution (5) in our derivation is still only valid for small  $u_{pi}$ . The conditional distribution (II.8) derived in the Appendix, however, is more general than (5) since it holds for any  $u_{p1} \neq 1$ ,  $u_{p2} \neq 1$  and small  $u_{p3}$ .

### Resolution of the sign ambiguity in single isomorphous replacement

Let the structure factors of the native, derivative and replacement structure in single isomorphous replacement (SIR) be denoted by  $F_i$ ,  $G_i$  and  $F'_i$  and the phases of  $F_i$  and  $F'_i$  by  $\varphi_i$  and  $\varphi'_i$ . With SIR data the following sign ambiguity remains if the replacement structure is known:

$$\varphi_i = \varphi'_i \pm |\Delta\varphi_i|, \quad (6)$$

where  $\Delta\varphi_i$  is defined as  $\Delta\varphi_i \equiv \varphi_i - \varphi'_i$  and its magnitude is calculated from

$$\cos |\Delta\varphi_i| = \frac{(-|F_i|^2 + |G_i|^2 - |F'_i|^2)}{2|F_i||F'_i|}. \quad (7)$$

Fan Hai-fu *et al.* (1984) proposed to resolve the sign ambiguity by calculating the probability that the sign of  $\Delta\varphi_i$  is positive *via* the Cochran distribution.

Fan Hai-fu *et al.* (1985) used the product of the Cochran distribution and Sim's (1959) distribution to incorporate partial structure information in the sign probability. In their procedure, correlations between the structure factors of a triple product are lost since Sim's distribution involves a single structure factor instead of three triple-related structure factors. We will solve this problem by calculating the sign probability *via* our distribution (4). Klop *et al.* (1987) suggested incorporation of partial structure information into the sign probability *via* Hauptman's (1982) joint probability distribution for the SIR case. The procedure adopted in the present paper, however, is to be preferred since other types of prior information can be exploited and the resolution dependence of the distribution parameters is now taken into account (*e.g.*  $Q'_{123}$  depends on  $\mathbf{h}_1$ ,  $\mathbf{h}_2$  and  $\mathbf{h}_3$ ).

Let part of the native structure, with normalized structure-factor magnitude  $u_{pi}$  and phase  $\beta_{pi}$ , be known. From the definitions  $\Delta\varphi_i \equiv \varphi_i - \varphi'_i$  and  $\delta_i \equiv \beta_{pi} - \varphi'_i$  we have  $\varphi_i = \beta_{pi} - \delta_i + \Delta\varphi_i$ . The phases  $\beta_{pi}$  and  $\delta_i$  are known and so is the magnitude  $|\Delta\varphi_i|$ .

Hence, the value of  $\varphi_i$  in (4) is  $\beta_{p_i} - \delta_i + |\Delta\varphi_i|$  or  $\beta_{p_i} - \delta_i - |\Delta\varphi_i|$ .

After substitution of  $\varphi_i$  in (4) by  $\beta_{p_i} - \delta_i + \Delta\varphi_i$  the joint probability distribution  $P(\Delta\varphi_1, \Delta\varphi_2, \Delta\varphi_3, R_1, R_2, R_3)$  can be obtained. This distribution can be used to derive the distribution  $P(\Delta\varphi_1 | R_1, R_2, R_3, |\Delta\varphi_2|, |\Delta\varphi_3|)$  or the distribution  $P(\Delta\varphi_1 | R_1, R_2, R_3, \Delta\varphi_2, \Delta\varphi_3)$ . With the definition  $\Phi' \equiv \varphi'_1 + \varphi'_2 + \varphi'_3$ , the latter distribution reads

$$P(\Delta\varphi_1 | R_1, R_2, R_3, \Delta\varphi_2, \Delta\varphi_3) \\ \sim \exp \{ [2R_1 u_{p1} / (1 - u_{p1}^2)] \cos(\Delta\varphi_1 - \delta_1) \\ + 2Q'_{123} / [(1 - u_{p1}^2)(1 - u_{p2}^2)(1 - u_{p3}^2)] \\ \times [R_1 R_2 R_3 \cos(\Delta\varphi_1 + \Delta\varphi_2 + \Delta\varphi_3 + \Phi' - q'_{123}) \\ - R_1 u_{p2} R_3 \cos(\Delta\varphi_1 + \delta_2 + \Delta\varphi_3 + \Phi' - q'_{123}) \\ - R_1 R_2 u_{p3} \cos(\Delta\varphi_1 + \Delta\varphi_2 + \delta_3 + \Phi' - q'_{123}) \\ + R_1 u_{p2} u_{p3} \cos(\Delta\varphi_1 + \delta_2 + \delta_3 + \Phi' - q'_{123})] \} \quad (8)$$

and is useful if the signs of the phase differences  $\Delta\varphi_2$  and  $\Delta\varphi_3$  have already been determined. This distribution replaces the product of the Cochran distribution and Sim's distribution used by Fan Hai-fu & Gu Yuan-xin (1985). The sign probability of  $\Delta\varphi_1$  that is obtained from (8) is denoted as  $\mathcal{P}_{\pm}(\Delta\varphi_1)$  and reads

$$\mathcal{P}_{\pm}(\Delta\varphi_1) = \frac{1}{2} \pm \frac{1}{2} \tanh(\sin(|\Delta\varphi_i|) \\ \times \{ [2R_1 u_{p1} / (1 - u_{p1}^2)] \sin \delta_1 \\ - 2Q'_{123} / [(1 - u_{p1}^2)(1 - u_{p2}^2)(1 - u_{p3}^2)] \\ \times [R_1 R_2 R_3 \sin(\Delta\varphi_2 + \Delta\varphi_3 + \Phi' - q'_{123}) \\ - R_1 u_{p2} R_3 \sin(\delta_2 + \Delta\varphi_3 + \Phi' - q'_{123}) \\ - R_1 R_2 u_{p3} \sin(\Delta\varphi_2 + \delta_3 + \Phi' - q'_{123}) \\ + R_1 u_{p2} u_{p3} \sin(\delta_2 + \delta_3 + \Phi' - q'_{123})] \} \}. \quad (9)$$

Identify  $\mathbf{h}_1$ ,  $\mathbf{h}_2$  and  $\mathbf{h}_3$  with  $-\mathbf{h}$ ,  $\mathbf{k}$  and  $\mathbf{h} - \mathbf{k}$ , respectively, and allow only partial structure information (i.e.  $q'_{123} = 0$ ), to compare (9) with the sign probability  $P_{\pm}(\Delta\varphi_{\mathbf{h}})$  (15) derived by Fan Hai-Fu & Gu Yuan-xin (1985). The last three sine terms in (9) of the present paper are missing in (15). Since  $\delta_1 = -\delta_{\mathbf{h}}$ ,  $\mathcal{P}_{-}(\Delta\varphi_{\mathbf{h}}) = \mathcal{P}_{+}(\Delta\varphi_{-\mathbf{h}})$  and  $\mathcal{P}_{+}(\Delta\varphi_{\mathbf{h}}) = \mathcal{P}_{-}(\Delta\varphi_{-\mathbf{h}})$ , the remaining terms of  $\mathcal{P}_{\pm}(\Delta\varphi_{\mathbf{h}})$  have the same sign as  $P_{\pm}(\Delta\varphi_{\mathbf{h}})$  of

Fan Hai-fu & Gu Yuan-xin (1985), but the coefficients differ. The latter formula is an approximation of (9) valid for small partial structures only, since the extra sine terms in (9) will in general not be negligible if partial structure information is available.

### Concluding remarks

The use of structural information in phase determination was shown by several authors to lead to better results. In a preliminary test (Main, 1976), the use of molecular structure was reported to lead to smaller root-mean-square errors in the estimated phases of triplet invariants. Camalli, Giacobazzo & Spagna (1985) demonstrated that several *MULTAN*-resistant structures can be solved easily by the use of partial structure information. Fan Hai-fu & Gu Yuan-Xin (1985) demonstrated that the sign ambiguity in single isomorphous replacement can be solved more easily if partial structure information is used.

We feel that a single theory which takes account of different types of structural information increases understanding and facilitates future applications. Therefore in the present paper the theoretical approaches of Main (1976), Heinerman (1977) and Giacobazzo (1983) are combined. We employed the resulting joint probability distribution to resolve the sign ambiguity in single isomorphous replacement; these results turn out to be valid regardless of the size of the partial structure.

### References

- CAMALLI, M., GIACOVAZZO, C. & SPAGNA, R. (1985). *Acta Cryst.* **A41**, 605-613.  
 COCHRAN, W. (1955). *Acta Cryst.* **8**, 473-478.  
 FAN HAI-FU & GU YUAN-XIN (1985). *Acta Cryst.* **A41**, 280-284.  
 FAN HAI-FU, HAN FU-SON, QIAN JIN-ZI & YAO JIA-XING (1984). *Acta Cryst.* **A40**, 489-495.  
 GIACOVAZZO, C. (1983). *Acta Cryst.* **A39**, 685-692.  
 HAO QUAN & FAN HAI-FU (1988). *Acta Cryst.* **A44**, 379-382.  
 HAUPTMAN, H. (1982). *Acta Cryst.* **A38**, 289-294.  
 HEINERMAN, J. J. L. (1977). *Acta Cryst.* **A33**, 100-106.  
 KLOP, E. A., KRABBENDAM, H. & KROON, J. (1987). *Acta Cryst.* **A43**, 810-820.  
 MAIN, P. (1976). In *Crystallographic Computing Techniques*, edited by F. R. AHMED, pp. 97-105. Copenhagen: Munksgaard.  
 SIM, G. A. (1959). *Acta Cryst.* **12**, 813-815.