Acta Cryst. (1983). A**39**, 273–277

Patterson Derivation of Structure Invariants: a Numerical Test

BY S. BRÜCKNER AND G. ALLEGRA

Dipartimento di Chimica, Politecnico di Milano, Piazza L. da Vinci 32, 20133 *Milano, Italy*

(*Received* 13 *April* 1982; *accepted* 20 *October* 1982)

Abstract

A numerical test is carried out on the theory proposed by one of the authors [Allegra (1979). *Acta Cryst.* A**35**, 213–220], which derives three-phase invariants from the Patterson function. The method is checked with two structures already solved ($P\bar{1}$ space group). For the strong Sayre triples the calculated cosine invariants are generally positive; the negative invariants arise from relatively minor features of the Patterson background, and so are more difficult to obtain. With a suitable choice both of the error standard deviation and of the degree of sharpening of the Patterson function, the average value of the calculated cosine invariants within small subsets of Sayre triples is reasonably close to +1, while that of the negative invariants is either smaller and positive or slightly negative. The agreement between the test calculations and the results obtained after structural refinement is much improved if the calculated amplitudes and an extended limiting sphere are used instead of the experimental data.

Foreword

In 1979 a theory was proposed by one of us that correlates the three-phase invariants with the Patterson function $P(\mathbf{u})$. It was shown first that $P^2(\mathbf{u})$ is proportional to the mean-square structure factor of a hypothetical structure obtained by self-multiplying the actual electron density after a translation $\mathbf{u}$ (the 'product' structure). Hence through least-squares considerations three-phase cosine and sine invariants are correlated with the Fourier components of the function $[P(\mathbf{u})]^{-2}$ (Allegra, 1979). Accordingly, the low-valued Patterson regions contribute most of the information, and this suggests that there may be a strong influence of the experimental errors on the results. As well as undertaking experimental checks on a new theory, this consideration prompted us to compare our calculations with the data of previously solved structures. We chose to limit our attention to the $P\bar{1}$ space group: this permits a non-trivial test on the negative cosine invariants, without taking advantage of peculiar symmetry effects.

Computational procedure

The three-phase cosine invariants are derived from a set of inhomogeneous linear equations, each set comprising in principle all triples involving one particular 'pivot' reflection, the reciprocal vector of which is $\mathbf{H}$. The jth equation of the related system, associated with the reciprocal vector $\mathbf{K}_j$, reads

$$\sum_i [2 - \delta(\mathbf{H} - 2\mathbf{K}_i)]|F_{\mathbf{K}_i} F_{\mathbf{H}-\mathbf{K}_i}|(Q_{\mathbf{H}-\mathbf{K}_i-\mathbf{K}_j} + Q_{\mathbf{K}_i-\mathbf{K}_j}) \times \cos(\varphi_{-\mathbf{H}} + \varphi_{-\mathbf{K}_i} + \varphi_{\mathbf{H}+\mathbf{K}_i}) = -2|F_0 F_{\mathbf{H}}|(Q_{\mathbf{H}-\mathbf{K}_j} + Q_{\mathbf{k}_j}), \quad (1)$$

where δ is the Kronecker delta. The meaning of $Q_{\mathbf{K}}$ is

$$Q_{\mathbf{K}} = \int_V \frac{1}{\langle \bar{P}^2(\mathbf{u})\rangle} \cos(2\pi \mathbf{K}.\mathbf{u})\, \mathrm{d}^3\mathbf{u}, \quad (2)$$

where $\langle \bar{P}^2(\mathbf{u})\rangle$ stands for 'best estimate of the square of the Patterson function $P(\mathbf{u})$' at the vector point u within the unit-cell volume V. In actual practice, if the calculated value $P(\mathbf{u})$ is sufficiently larger than zero we have

$$\langle \bar{P}^2(\mathbf{u})\rangle = P^2(\mathbf{u}) + \sigma_P^2 \quad (3)$$

where σ_P^2, *i.e.* the error variance of $P(\mathbf{u})$, is assumed to be constant throughout the unit cell. If $P(\mathbf{u})$ is very close to or smaller than zero a more general statistical criterion is needed to evaluate $\langle \bar{P}^2(\mathbf{u})\rangle$ (see Allegra, 1979, Fig. 1). Although the *a priori* evaluation of σ_P appears to be rather difficult, we decided to take it of the same order of magnitude as the lowest value of the Patterson function, see following. It should be pointed out that in system (1) the only unknowns are the cosine invariants, all the remaining quantities being derivable from the observed amplitudes.

Indicating with $c_{\mathbf{H}}(i)$ the cosine invariant $\cos(\varphi_{-\mathbf{H}} + \varphi_{\mathbf{K}_i} + \varphi_{\mathbf{H}-\mathbf{K}_i})$ within system (1), from an analysis of the coefficients $Q_{\mathbf{K}}$ and assuming all the three amplitudes $|F_{\mathbf{H}}|$, $|F_{\mathbf{K}_i}|$ and $|F_{\mathbf{H}-\mathbf{K}_i}|$ to be large, it was suggested that the coefficient of the diagonal element $c_{\mathbf{H}}(j)$ should be usually very large and positive, while the constant term on the right-hand side should also be large and positive. In conclusion, the most probable sign of $c_{\mathbf{H}}(j)$ is positive if the three amplitudes contributing to the

0567-7394/83/030273-05$01.50 © 1983 International Union of Crystallography

triple are large, in agreement with the current statistical theories. Accordingly, it is a reasonable expectation that if any cosine invariant is to be negative, relatively minor details of the low-valued Patterson regions should concur to determine its negative value from system (1).

From our numerical analysis, details of this sort are strongly influenced by the following factors: (i) the experimental error of the observed amplitudes; (ii) the series truncation in the evaluation of $P(\mathbf{u})$; (iii) the choice of σ_P; (iv) the (possible) degree of sharpening of $P(\mathbf{u})$. As for the last item, we have used the following procedure to build up a partially sharpened Patterson function. Let Z_l and $f_l(\mathbf{H})$ respectively be the atomic number of the lth atom and its scattering factor at the reciprocal point $\mathbf{H}$. If p is a parameter between zero and unity, defining

$$g_l(\mathbf{H}) = (1-p)\,Z_l + p f_l(\mathbf{H}), \qquad (4)$$

the coefficients of the partially sharpened Patterson function are

$$\hat{P}^2_{\mathbf{H}} = F^2_{\mathbf{H}} \frac{\sum_l Z_l^2}{\sum_l g_l^2(\mathbf{H})},$$

where the sums are extended to all the atoms within the unit cell. It is easy to verify that by setting $p = 1$ we have a completely sharpened function, *i.e.* the contributing atoms are (approximately) reduced to point-like entities, while for $p = 0$ the usual Patterson coefficients are employed. A large value of p may expand the background details that are important for our purposes, but it may inflate the error and truncation effects at the same time; search for a compromise is one of the scopes of the present investigation.

Numerical results and discussion

Two previously solved structures were used in our calculations, namely that of the *A-cis'-cis* stereoisomer of dodecahydrotriptycene (Albinati, Brückner & Allegra, 1977; structure *A*) and that of 2-*exo*-(2-methylallyl)norbornane-3-*exo*-carboxylic acid (Albinati, Zocchi, Germain & Declercq, 1973; structure *B*), both of which belong to the $P\bar{1}$ space group, as anticipated. The two structures respectively contain a total of 40 and 28 C + O atoms within the unit cell.

Each system of linear equations like (1), based on any selected reciprocal vector $\mathbf{H}$, may produce many cosine invariants; in our cases an average of about one hundred significant invariants per basic reflection was obtained. Consequently, instead of giving all the results in detail we decided to show the average values of the invariants grouped within subsets according to the value of $|E_{-\mathbf{H}}E_{\mathbf{K}}E_{\mathbf{H}-\mathbf{K}}|$, *limiting our analysis to the reflections with* $|E| > 1$. The subsets were constructed as given in Table 1, and the average values will be given separately for the cosine invariants known to be positive and for those known to be negative. Also, we will compare the results obtained from functions $\langle \tilde{P}^2(\mathbf{u}) \rangle$ [see (2)] evaluated under different conditions, with the purpose of testing the effects of the factors (i) to (iv) listed in the previous section.

Table 2 reports some results obtained with the same degree of sharpening [$p = 0{\cdot}8$, see (4)] and with three different values of σ_p for both structures. The figure selected for p appeared to represent the best compromise between the contrasting requirements discussed in the previous section. Calculated cosines outside the allowed range (−1)–(+1) may appear for low σ_p's; conversely, for high σ_p's they tend to assume uniform values much smaller than unity. These observations agree with the conclusion that inadequate account of the experimental error (*i.e.* too low a σ_p) may lead to erratic results while allowing for too wide error limits (high σ_p) may wipe out all the relevant information. As expected, the calculated cosines tend to be positive even when referring to a triple known to be negative, although they are smaller in this case than the corresponding cosines of positive triples, with virtually no exception.

Table 3 shows a comparison for both structures between the results obtained for various degrees of sharpening p although with a fixed σ_p. Remembering that a strong sharpening emphasizes the details, therefore corresponding to the effect of a low σ_p, the results of Table 2 produce information analogous to that extracted from Table 1. The value $p = 0{\cdot}8$ appears to lead to optimal results in both cases.

Table 4 shows the effect of the random errors, in addition to that of series truncation, for both structures. The cosine invariants calculated from the observed amplitudes, truncated at a minimum spacing $d_{\min} = 0{\cdot}9$ Å, are compared with those derived from the calculated amplitudes, with $d_{\min} = 0{\cdot}6$ Å; the same values of σ_p and p are applied to both Patterson maps. As expected, the maps from the calculated amplitudes give a much better prediction for the negative cosine invariants.

A deeper analysis was applied to results obtained with $\sigma_p = 60$ e² Å^{-3} and $p = 0{\cdot}8$ for structure *A* and $\sigma_p = 20$ e² Å^{-3} and $p = 0{\cdot}8$ for structure *B*, *i.e.* the values of σ_p and p giving estimated average cosines of order unity without great departures of single values from the mean (the calculated cosines range rather uniformly from −0·2 to 1·2). Results are reported in

Table 1. *Definition of the subsets of the triples according to the value of* $|E_{-\mathbf{H}}.E_{\mathbf{K}}.E_{\mathbf{H}-\mathbf{K}}|$

Type of subset	1	2	3	4	5
Range of $\|E_{-\mathbf{H}}.E_{\mathbf{K}}.E_{\mathbf{H}-\mathbf{K}}\|$	>20	14–20	9–14	6–9	<6

Table 2. *Some results from structures A and B (see text)*

Each section summarizes the results from the system of linear equations based on the reflection indicated at the top, together with its E value in parentheses. Triples are classified into five subsets (see first column) according to the value of $|E_{-H}E_{K}E_{H-K}|$, see Table 1. Within each subset the triples known to be positive (+) are separated from those known to be negative (−). Under each (+, −) label three columns report average values of C_H(i)'s corresponding to the three values of σ_p used in the calculation (e² Å^{-3}), see text. Numbers in parentheses indicate how many triples contribute to the average. The parameter p is set equal to 0·8.

Structure *A*

		(+)			(−)			
Subset	σ_p	40	60	80	σ_p	40	60	80
Reflection 6 −5 1 (E = 6·55)								
1	(69)	2·278	1·289	1·115	/	/	/	/
2	(26)	−0·1222	0·686	0·770	/	/	/	/
3	(1)	0·696	0·976	0·964	/	/	/	/
Reflection 2 8 0 (E = 4·05)								
1	(23)	1·129	0·818	0·728	/	/	/	/
2	(23)	1·375	0·838	0·748	/	/	/	/
3	(22)	1·054	0·736	0·674	/	/	/	/
Reflection 0 6 0 (E = 3·01)								
1	(9)	1·037	0·773	0·672	/	/	/	/
2	(6)	1·075	0·725	0·623	/	/	/	/
3	(30)	1·138	0·678	0·600	(1)	0·341	0·184	0·200
4	(7)	0·754	0·414	0·379	(2)	−1·122	−0·292	−0·116
Reflection 1 2 1 (E = 2·80)								
1	(7)	1·276	1·032	0·927	/	/	/	/
2	(8)	0·906	0·855	0·790	/	/	/	/
3	(17)	1·198	0·847	0·771	/	/	/	/
4	(20)	0·634	0·687	0·637	(1)	0·062	0·377	0·391
5	(11)	1·310	0·798	0·674	(1)	0·791	0·176	0·183
Reflection 4 −1 1 (E = 2·80)								
1	(7)	1·018	0·845	0·762	/	/	/	/
2	(10)	1·333	0·918	0·814	(1)	0·491	0·434	0·410
3	(22)	0·671	0·594	0·567	(2)	0·771	0·512	0·486
4	(7)	0·757	0·591	0·525	(5)	0·758	0·688	0·613
5	(3)	1·743	0·948	0·632	(3)	0·316	0·328	0·334
Reflection −1 0 1 (E = 2·40)								
1	(6)	1·230	1·121	0·945	/	/	/	/
2	(6)	2·050	0·932	0·874	/	/	/	/
3	(19)	2·130	0·954	0·874	(1)	0·712	0·741	0·783
4	(22)	1·846	0·835	0·750	(1)	−2·247	0·012	0·026
5	(16)	2·036	0·743	0·638	(3)	1·492	0·314	0·182
Reflection −2 0 2 (E = 2·06)								
1	(1)	1·671	1·423	1·238	/	/	/	/
2	(2)	1·117	1·037	0·928	/	/	/	/
3	(8)	1·086	0·829	0·712	(2)	−0·015	0·379	0·401
4	(18)	0·567	0·564	0·523	(4)	0·379	0·283	0·278
5	(21)	0·564	0·477	0·434	(3)	0·398	0·051	0·078

Structure *B*

		(+)			(−)			
Subset	σ_p	20	40	100	σ_p	20	40	100
Reflection −1 0 1 (E = 3·00)								
1	(1)	1·132	0·841	0·625	/	/	/	/
2	(11)	1·197	0·818	0·638	/	/	/	/
3	(16)	1·166	0·912	0·623	/	/	/	/
4	(30)	1·030	0·791	0·581	/	/	/	/
5	(28)	1·070	0·744	0·520	(4)	0·109	0·132	0·229
Reflection 2 −3 1 (E = 2·40)								
1	(1)	0·806	0·617	0·423	/	/	/	/
2	(3)	0·962	0·634	0·448	/	/	/	/
3	(7)	0·710	0·588	0·404	/	/	/	/
4	(22)	0·824	0·597	0·416	(2)	0·713	0·588	0·444
5	(34)	0·686	0·431	0·342	(4)	0·341	0·301	0·284
Reflection 3 −2 2 (E = 1·80)								
3	(5)	0·688	0·594	0·318	/	/	/	/
4	(10)	0·638	0·578	0·313	/	/	/	/
5	(43)	0·575	0·417	0·254	(7)	0·341	0·281	0·152
Reflection 2 −1 1 (E = 1·66)								
3	(1)	0·535	0·481	0·304	/	/	/	/
4	(10)	0·650	0·521	0·325	/	/	/	/
5	(43)	0·558	0·417	0·271	(18)	0·187	0·190	0·193
Reflection 1 0 0 (E = 1·02)								
4	(2)	0·448	0·384	0·271	/	/	/	/
5	(50)	0·402	0·318	0·248	(11)	0·187	0·182	0·174

Table 5 where the calculated cosines are grouped into five subsets according to their values and for each subset the number of known positive triples and the number of known negative triples are indicated. This table shows that the magnitude of the calculated cosines is itself a rough measure of confidence of their sign (provided there are no great distorsions due to a bad choice of σ_P and p).

Table 3. *Some results from structures A and B*

The effect of an increasing sharpening of the Patterson function is reported. Parameter σ_P is set equal to 60 and 20 e² Å^{-3} respectively.

Structure *A*

		(+)			(−)		
Subset	p	0·0	0·8	1·0	p	0·0	0·8	1·0
Reflection 6 −5 1								
1	(69)	0·664	1·289	0·081	/	/	/	/
2	(26)	0·659	0·686	−1·969	/	/	/	/
3	(1)	0·486	0·976	−6·204	/	/	/	/
Reflection 2 8 0								
1	(23)	0·393	0·818	−0·144	/	/	/	/
2	(23)	0·352	0·838	0·297	/	/	/	/
3	(22)	0·273	0·736	0·137	/	/	/	/
Reflection 0 6 0								
1	(9)	0·397	0·773	−3·082	/	/	/	/
2	(6)	0·386	0·725	−0·008	/	/	/	/
3	(30)	0·374	0·678	−13·766	(1)	0·243	0·184	1·941
4	(7)	0·397	0·414	−1·464	(2)	0·186	−0·292	0·818
Reflection 1 2 1								
1	(7)	0·598	1·032	3·141	/	/	/	/
2	(8)	0·581	0·855	−2·183	/	/	/	/
3	(17)	0·678	0·847	0·103	/	/	/	/
4	(20)	0·534	0·687	2·321	(1)	0·410	0·377	−2·131
5	(11)	0·359	0·798	4·630	(1)	0·068	0·176	1·184
Reflection 4 −1 1								
1	(7)	0·533	0·845	−3·895	/	/	/	/
2	(10)	0·565	0·918	2·797	(1)	0·489	0·434	−1·333
3	(22)	0·522	0·594	−4·322	(2)	0·557	0·512	1·386
4	(7)	0·523	0·591	4·718	(5)	0·550	0·688	2·264
5	(3)	0·335	0·948	−1·519	(3)	0·228	0·328	−2·924
Reflection −1 0 1								
1	(6)	1·195	1·121	0·459	/	/	/	/
2	(6)	1·333	0·932	−0·294	/	/	/	/
3	(19)	1·173	0·954	0·152	(1)	0·821	0·741	−0·095
4	(22)	0·999	0·835	0·277	(1)	0·979	0·012	0·004
5	(16)	0·865	0·743	0·011	(3)	0·505	0·314	0·026
Reflection −2 0 2								
1	(1)	0·631	1·423	−1·413	/	/	/	/
2	(2)	0·658	1·037	2·818	/	/	/	/
3	(8)	0·487	0·829	3·421	(2)	0·302	0·379	0·555
4	(18)	0·424	0·564	−3·884	(4)	0·557	0·283	−2·034
5	(21)	0·299	0·477	2·418	(3)	0·204	0·051	3·592

Structure *B*

		(+)			(−)		
Subset	p	0·5	0·8		p	0·5	0·8
Reflection −1 0 1							
1	(1)	1·050	1·132	/	/	/	
2	(11)	1·077	1·197	/	/	/	
3	(16)	1·025	1·166	/	/	/	
4	(30)	0·965	1·030	/	/	/	
5	(28)	0·964	1·070	(4)	0·027	0·109	
Reflection 2 −3 1							
1	(1)	0·710	0·806	/	/	/	
2	(3)	0·874	0·962	/	/	/	
3	(7)	0·576	0·710	/	/	/	
4	(22)	0·731	0·824	(2)	0·648	0·713	
5	(34)	0·631	0·686	(4)	0·296	0·341	
Reflection 3 −2 2							
3	(5)	0·500	0·688	/	/	/	
4	(10)	0·625	0·638	/	/	/	
5	(43)	0·456	0·575	(7)	0·263	0·044	
Reflection 2 −1 1							
3	(1)	0·455	0·535	/	/	/	
4	(10)	0·672	0·650	/	/	/	
5	(43)	0·468	0·558	(18)	0·250	0·197	
Reflection 1 0 0							
4	(2)	0·399	0·448	/	/	/	
5	(50)	0·366	0·402	(11)	0·207	0·187	

Table 4. *Some results in structures A and B (see text and Table 2)*

Comparison between calculations carried out with F_{obs}'s and with F_{calc}'s. The latter have been calculated up to $\sin\theta/\lambda \simeq 0{\cdot}80$. Parameter p is set equal to 0·8 while σ_p is equal to 60 e² Å^{-3} in structure *A* and 20 e² Å^{-3} in structure *B*. Numbers in parentheses indicate how many triples contribute to the given average.

Structure *A*

	(+)		(−)	
Subset	Observed	Calculated	Observed	Calculated
Reflection 6 −5 1				
1	1·289 (69)	0·695 (110)	/	/
2	0·686 (26)	/	/	/
3	0·976 (1)	/	/	/
Reflection 1 2 1				
1	1·032 (7)	0·945 (14)	/	/
2	0·855 (8)	0·851 (14)	/	/
3	0·847 (17)	0·682 (28)	/	/
4	0·687 (20)	0·576 (32)	0·377 (1)	−0·011 (2)
5	0·798 (11)	0·011 (4)	/	/
Reflection 4 −1 1				
1	0·845 (7)	0·746 (12)	/	/
2	0·918 (10)	0·629 (11)	/	/
3	0·594 (22)	0·471 (27)	0·312 (2)	0·062 (2)
4	0·591 (7)	0·337 (17)	0·295 (4)	0·092 (4)
5	0·948 (3)	0·332 (7)	/	/
Reflection −1 0 1				
1	1·121 (6)	0·922 (12)	/	/
2	0·932 (6)	0·836 (15)	/	/
3	0·954 (19)	0·664 (33)	0·741 (1)	0·015 (1)
4	0·835 (22)	0·661 (41)	0·012 (1)	−0·293 (4)
5	0·743 (16)	0·276 (4)	0·314 (3)	−0·204 (4)

Structure *B*

	(+)		(−)	
Subset	Observed	Calculated	Observed	Calculated
Reflection −1 0 1				
1	0·841 (1)	1·181 (5)	/	/
2	0·818 (11)	0·919 (19)	/	/
3	0·912 (16)	0·985 (24)	/	/
4	0·791 (30)	0·931 (32)	/	/
5	0·744 (28)	0·845 (25)	0·132 (4)	0·010 (7)
Reflection 2 −3 1				
1	0·618 (1)	0·748 (8)	/	/
2	0·634 (3)	0·780 (12)	/	/
3	0·588 (7)	0·810 (17)	/	/
4	0·597 (22)	0·748 (32)	/	0·043 (1)
5	0·431 (34)	0·702 (35)	0·281 (7)	0·341 (10)
Reflection 2 −1 1				
3	0·481 (1)	0·856 (4)	/	/
4	0·521 (10)	0·965 (22)	/	0·223 (2)
5	0·417 (43)	0·756 (38)	0·190 (18)	0·219 (25)
Reflection 1 0 0				
4	0·384 (2)	0·544 (16)	/	0·143 (3)
5	0·318 (50)	0·531 (58)	0·182 (11)	0·260 (16)

Concluding remarks

The satisfactory degree of discrimination between positive and negative triples within small subsets in the $P\bar{1}$ space group, in spite of a few individual wrong predictions, suggests that the present approach may lead to a useful new figure of merit for multisolution methods. More generally, the present approach seems to offer an alternative way to the classical statistical derivation of three-phase invariants (Cochran, 1955; Hauptman, 1972; Giacovazzo, 1974). Of course it should be recalled for this purpose that new methods producing the statistical evaluation of high-order phase invariants (*e.g.* Hauptman, 1975; Giacovazzo, 1976*a*,*b*,*c*; Hauptman & Green, 1976; Giacovazzo, 1980) may also lead to negative cosine invariants in space groups with no translation symmetry elements.

Table 5. *Synthetic analysis of the results obtained for structures A and B when $\sigma_p = 60$ e² Å^{-3}, $p = 0{\cdot}8$ and $\sigma_p = 20$ e² Å^{-3}, $p = 0{\cdot}8$ are used respectively*

Distinction among 'pivot' reflections is omitted. Calculated triples are grouped according to their values within five subsets. For each subset the number of known positive triples and the number of known negative triples are indicated.

	Positive triples	Negative triples
Structure *A*		
Calculations based on seven 'pivot' reflections		
Subset *a* ($c_H > 1$)	96	1
Subset *b* ($0{\cdot}6 < c_H < 1{\cdot}0$)	207	1
Subset *c* ($0{\cdot}3 < c_H < 0{\cdot}6$)	99	12
Subset *d* ($0 < c_H < 0{\cdot}3$)	36	11
Subset *e* ($c_H < 0$)	9	5
Structure B		
Calculations based on six 'pivot' reflections		
Subset *a* ($c_H > 1$)	66	1
Subset *b* ($0{\cdot}6 < c_H < 1$)	159	8
Subset *c* ($0{\cdot}3 < c_H < 0{\cdot}6$)	103	18
Subset *d* ($0 < c_H < 0{\cdot}3$)	33	14
Subset *e* ($c_H < 0$)	13	20

References

ALBINATI, A., BRÜCKNER, S. & ALLEGRA, G. (1977). *Acta Cryst.* B**33**, 229–231.

ALBINATI, A., ZOCCHI, M., GERMAIN, G. & DECLERCQ, J. P. (1973). *Cryst. Struct. Commun.* **2**, 585–587.

ALLEGRA, G. (1979). *Acta Cryst.* A**35**, 213–220.

COCHRAN, W. (1955). *Acta Cryst.* **8**, 473–478.

GIACOVAZZO, C. (1974). *Acta Cryst.* A**30**, 757–761.

GIACOVAZZO, C. (1976*a*). *Acta Cryst.* A**32**, 91–99.

GIACOVAZZO, C. (1976*b*). *Acta Cryst.* A**32**, 100–104.

GIACOVAZZO, C. (1976*c*). *Acta Cryst.* A**32**, 958–966.

GIACOVAZZO, C. (1980). *Direct Methods in Crystallography*. New York: Academic Press.

HAUPTMAN, H. (1972). *Z. Kristallogr.* **135**, 1–8.

HAUPTMAN, H. (1975). *Acta Cryst.* A**31**, 671–679.

HAUPTMAN, H. & GREEN, E. A. (1976). *Acta Cryst.* A**32**, 45–49.