

sides of a strip. As a consequence, the new surfaces form two different kinds of channels parallel to the strips, whereas the *CLP*, *oCLP*, *tD*, *oDa* and *oDb* surfaces form only one kind each.

In contrast to minimal balance surfaces generated from catenoids, branched catenoids and multiple catenoids, minimal surfaces that may be generated from strip-like surface patches seem not to be restricted with respect to the axial ratio c/a . Apparently the distance between the rectangular nets may grow arbitrarily large. This property is not surprising with respect to those minimal surfaces that may be generated also from disc-like surface patches. With respect

to *ST1* and *ST2* surfaces the following idea may be helpful: a strip-like surface patch approximates in its central part more and more to a plane if the distance between its two boundaries becomes wider and wider.

References

- BOHM, J. & DORNBERGER-SCHIFF, K. (1967). *Acta Cryst.* **23**, 913-933.
 FISCHER, W. & KOCH, E. (1987). *Z. Kristallogr.* **179**, 31-52.
 FISCHER, W. & KOCH, E. (1989). *Acta Cryst.* **A45**, 166-169.
 KOCH, E. & FISCHER, W. (1988). *Z. Kristallogr.* **183**, 129-152.
 KOCH, E. & FISCHER, W. (1989). *Acta Cryst.* **A45**, 169-174.
 SCHOEN, A. H. (1970). *Infinite Periodic Minimal Surfaces Without Self-Intersections*. NASA Tech. Note No. D-5541.

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A Geometrically Constrained Phase Refinement Function: the Derivation of a New Modified Tangent Formula

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Abstract

A new phase refinement function that makes explicit use of the well resolved nature of the atomic peaks is presented. This function is first deduced for the one-dimensional case and then extended to the three-dimensional one. A new modified tangent formula can be derived from it. The effectiveness of this modified tangent formula is illustrated on the basis of some test structures. This function also seems to provide the *XYM* function of Debaerdemaeker & Woolfson [*Acta Cryst.* (1983), **A39**, 193-196] with a possible rational explanation.

1. Introduction

As a logical consequence of the availability of faster computers, a number of new multisolution direct methods have been developed in the last years for refining initially random sets of phases, e.g. the *YZARC* method of Baggio, Woolfson, Declercq & Germain (1978), the *RANTAN* approach of Yao Jia-xing (1981), the *XYM* function of Debaerdemaeker & Woolfson (1983) and more recently the Sayre (1952) equation tangent formula discussed by Debaerdemaeker, Tate & Woolfson (1985, 1988). Following this trend, a new method has been investigated. It is based on the maximization of a function that explicitly incorporates, besides the positivity, another general and important property of the elec-

tron density, i.e. the atomicity. It will be shown that the introduction of this additional constraint makes this function especially well suited for refining initially random sets of phases *via* a modified tangent formula.

2. The one-dimensional case

2.1. Derivation of the new phase refinement function

As is well known (Cochran, 1952), the integral

$$a^2 \int_a \rho^3(r) dr \quad (1)$$

must be a strong maximum, since $\rho(r)$, i.e. the electron density distribution of a one-dimensional model structure of cell period a , is positive and principally located at the atomic positions. On the other hand, if t represents a shift approximately equal to the average width of the atomic peaks, and since the atoms must be well resolved, then the integral

$$a^2 \int_a \rho(r+t)\rho^2(r) dr \quad (2)$$

will be small. Consequently, the difference between the two integrals, i.e. (1) - (2), should be a large positive value for the true structure. However, (2) becomes a large positive value for wrong $\rho(r)$ distributions containing poorly resolved peaks, i.e. peaks with widths greater than t . In these cases, the difference (1) - (2) will be smaller.

The new phase refinement function Ω to be maximized is defined for the one-dimensional case as

$$\Omega = a^2 \int_{\alpha} \rho^3(r) dr - pa^2 \int_{\alpha} \rho(r+t)\rho^2(r) dr \quad (3)$$

and, therefore, combines in a single expression two general properties of $\rho(r)$, *i.e.* the positivity and the atomicity, explicitly. Ω can only be a large maximum if (1) is large and positive and, simultaneously, (2) is small or slightly negative. The factor p allows one to modulate the weight of the integral (2) in (3) and is assumed to be unity in this paper.

A rather common cause for the failure of conventional direct methods consists of the overlap of the two enantiomers in the resulting E map (Debaerdemaeker, 1982). Consequently, a function like (3) that minimizes the presence of partially overlapped peaks should reduce the incidence of this cause.

If the atoms in $\rho(r)$ are assumed to be *point atoms*, then (3) may be approximated by means of the double summation

$$\begin{aligned} \Omega = & \sum_h \{1 - p \exp[-i2\pi(-h)t]\} \\ & \times \sum_{h'} |E_{-h}E_{h'}E_{h-h'}| \exp i\Phi_3 \end{aligned} \quad (4)$$

where $\mathbf{E}_h = E_h \exp i\varphi_h$ is the normalized structure factor of reflection h , $-2\pi(-h)t$ is the phase shift introduced by the translation t , and $\Phi_3 = \varphi_{-h} + \varphi_{h'} + \varphi_{h-h'}$. If

$$C_h = 1 - p \cos(-2\pi ht) \quad (5)$$

and

$$S_h = -p \sin(-2\pi ht) \quad (6)$$

then the first complex factor in (4) can be expressed in trigonometric form as

$$1 - p \exp[-i2\pi(-h)t] = W_{-h} \exp i\xi_{-h} \quad (7)$$

with

$$W_{-h} = [C_{-h}^2 + S_{-h}^2]^{1/2} \quad (8)$$

and

$$\tan \xi_{-h} = S_{-h}/C_{-h}. \quad (9)$$

If one substitutes (7) in (4), and since $W_h = W_{-h}$ and $\xi_h = -\xi_{-h}$, the real expression (10) follows, *i.e.*

$$\begin{aligned} \Omega = & \sum_h \sum_{h'} W_{-h} |E_{-h}E_{h'}E_{h-h'}| \exp i(\Phi_3 + \xi_{-h}) \\ = & \sum_h W_{-h} \sum_{h'} |E_{-h}E_{h'}E_{h-h'}| \cos(\Phi_3 + \xi_{-h}). \end{aligned} \quad (10)$$

By developing the cosine term in (10) and considering that $C_{-h} = W_{-h} \cos \xi_{-h}$ and $S_{-h} = W_{-h} \sin \xi_{-h}$, one obtains the following equivalent expression for Ω :

$$\Omega = \sum_h \sum_{h'} |E_{-h}E_{h'}E_{h-h'}| (C_{-h} \cos \Phi_3 - S_{-h} \sin \Phi_3). \quad (11)$$

If the shift were $-t$, the cosine term in (10) would be

$\cos(\Phi_3 - \xi_{-h})$ and the minus sign in (11) would become positive.

2.2. Practical example

A one-dimensional equal-atom structure with atoms at 0.00, 0.20, 0.50 and 0.75 in a cell of length 10 Å has been selected to illustrate the application of Ω using (10) (Fig. 1). The phase refinement method employed is very simple and consists of regarding the phase value φ_h that maximizes the corresponding internal summation h' in (10) as the refined one. This φ_h is then used in the phase refinement of the subsequent reflections.

The results of a series of consecutive refinements of initially random phase sets using this procedure (20 cycles each trial) are shown in Table 1. The correct and the refined phases of the triplets are given in Table 2. It can be seen how the refined phases of the triplets no longer tend towards zero. The significance of $v(h, h')$ and $\psi(h, h')$ in Table 2 will be explained in § 3.2.

3. The three-dimensional case

3.1. The Ω function for non-centrosymmetrical structures

The three-dimensional Ω function is defined in direct space by

$$\Omega = V^2 \int_V \rho^3(\mathbf{r}) d\mathbf{r} - pV^2 \int_V \rho_s(\mathbf{r})\rho^2(\mathbf{r}) d\mathbf{r} \quad (12)$$

where

$$\begin{aligned} \rho_s(\mathbf{r}) = & V^{-1} \sum_{\mathbf{k}} \sum_j \{ \mathbf{F}_{\mathbf{k}R_j} \exp[-i2\pi\mathbf{k}R_j(\mathbf{r} + R_j^{-1}\mathbf{t})] \\ & + \mathbf{F}_{-\mathbf{k}R_j} \exp[i2\pi\mathbf{k}R_j(\mathbf{r} + R_j^{-1}\mathbf{t})] \} \end{aligned} \quad (13)$$

$$\begin{aligned} = & V^{-1} \sum_{\mathbf{k}} \sum_j [\exp(-i2\pi\mathbf{k}\mathbf{t}) \mathbf{F}_{\mathbf{k}R_j} \exp(-i2\pi\mathbf{k}R_j\mathbf{r}) \\ & + \exp(i2\pi\mathbf{k}\mathbf{t}) \mathbf{F}_{-\mathbf{k}R_j} \exp(i2\pi\mathbf{k}R_j\mathbf{r})] \end{aligned} \quad (14)$$

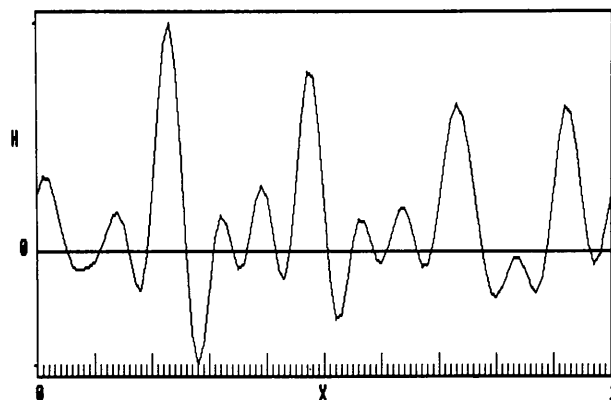


Fig. 1. One-dimensional E map of the one-dimensional model structure computed with nine phases refined with function Ω (mean phase error = 18°, $t = 0.55$ Å); H = height of the E synthesis in arbitrary units, x = fractional coordinates.

Table 1. Results of the Ω refinement function for the one-dimensional example

NPH = number of phases, NR = number of Σ_2 relationships, NT = number of trials and MPHE = mean phase error in degrees with e.s.d.'s in parentheses. $\{E_{\min} = 0.71, [(\sin \theta)/\lambda]_{\max} = 0.65 \text{ \AA}^{-1}, t = 0.55 \text{ \AA}\}$

NPH	NR	NT	MPHE			
9	36	20	15 (11)	16 (12)	16 (12)	20 (15)
			21 (17)	22 (18)	22 (19)	23 (20)
			24 (17)	28 (21)	28 (19)	34 (28)
			34 (25)	34 (27)	36 (26)	40 (35)
			41 (35)	42 (35)	43 (24)	44 (35)

Table 2. Values of $v(\mathbf{h}, \mathbf{h}')$ and $\psi(\mathbf{h}, \mathbf{h}')$ and the correct and refined phases of the strongest triplets

$-\mathbf{h}$	\mathbf{h}'	$\mathbf{h}-\mathbf{h}'$	$ E_3 $	$v(\mathbf{h}, \mathbf{h}')$	$\psi(\mathbf{h}, \mathbf{h}')$ ($^\circ$)	Φ_3 ($^\circ$)	$\Phi_{3\text{ref}}$ ($^\circ$)
-4	-9	13	1.5	1.5	-26	-20	20
-4	-8	12	2.2	1.6	-27	46	38
-4	-7	11	1.5	1.6	-27	-20	19
-4	-6	10	1.4	1.6	-27	-20	12
-4	-4	8	3.4	1.3	-24	17	57
-6	-7	13	0.6	1.7	-29	90	89
-6	-6	12	0.7	1.7	-30	-57	-10

where R_j is the matrix of the j th point-group symmetry operation; $R_j^{-1}\mathbf{t}$ gives the shifts of the electron-density peak; \mathbf{k} are reflections belonging to one asymmetric unit of the reciprocal space; and V is the cell volume. Physically, $\rho_s(\mathbf{r})$ represents an electron density function with the atomic peak modified in such a way that it is no longer spherical but splits up according to the shifts $R_j^{-1}\mathbf{t}$. This means that if the peaks are well resolved, then the electron density will not form a maximum at the centre of the peak, but will be concentrated at the ends of the vectors $R_j^{-1}\mathbf{t}$ and, therefore, the second integral in (12) will vanish.

However, if a wrong $\rho(\mathbf{r})$ distribution contains strong positive broad peaks, $\rho_s(\mathbf{r})$ will still be positive at their centres and, consequently, the second integral in (12) will be a strong positive quantity. This implies that the Ω function cannot be a positive maximum in this last case.

If one makes

$$W_{\mathbf{k}R_j} \exp(i\xi_{\mathbf{k}R_j}) = 1 - p \exp(-i2\pi\mathbf{k}\mathbf{t}) \quad (15a)$$

and

$$W_{-\mathbf{k}R_j} \exp(i\xi_{-\mathbf{k}R_j}) = 1 - p \exp(i2\pi\mathbf{k}\mathbf{t}) \quad (15b)$$

and after introduction of the E 's, the corresponding expression for the Ω function in reciprocal space is

$$\begin{aligned} \Omega(\mathbf{t}) &= \sum_{\mathbf{h}} W_{-\mathbf{h}} \exp(i\xi_{-\mathbf{h}}) \sum_{\mathbf{h}'} |E_{-\mathbf{h}} E_{\mathbf{h}'} E_{\mathbf{h}-\mathbf{h}'}| \exp i\Phi_3 \\ &= \sum_{\mathbf{h}} W_{-\mathbf{h}} \sum_{\mathbf{h}'} |E_{-\mathbf{h}} E_{\mathbf{h}'} E_{\mathbf{h}-\mathbf{h}'}| \cos(\Phi_3 + \xi_{-\mathbf{h}}) \quad (16) \end{aligned}$$

$$= \sum_{\mathbf{k}} m(\mathbf{k}) W_{-\mathbf{k}} \sum_{\mathbf{h}'} |E_{-\mathbf{k}} E_{\mathbf{h}'} E_{\mathbf{k}-\mathbf{h}'}| \cos(\Phi_3 + \xi_{-\mathbf{k}}), \quad (17)$$

where m is the multiplicity of \mathbf{k} .

An approximation to the Ω function may be obtained by replacing the two factors $m(\mathbf{k})$ and $W_{-\mathbf{k}}$ in (17) by a constant factor, as well as by substituting the proper $\xi_{-\mathbf{k}}$ values by an average one $\langle \xi_{-\mathbf{k}} \rangle$ defined as

$$\langle \xi_{-\mathbf{k}} \rangle = \frac{\sum_{\mathbf{k}} W_{-\mathbf{k}} \xi_{-\mathbf{k}}}{\sum_{\mathbf{k}} W_{-\mathbf{k}}}.$$

The values of $\langle \xi_{-\mathbf{k}} \rangle$ lie between -35 and -55° for the test examples given in § 3.3. It is interesting to note that this approximation is similar to the empirically found XMY function of Debaerdemaeker & Woolfson (1983).

3.2. How to maximize the Ω function?

The Ω function as given in (17) can be maximized using the parameter-shift refinement procedure (Bhuiya & Stanley, 1963). This method has been adapted to phase refinement by Debaerdemaeker (1982) and is very useful for complicated functions. On the other hand, it is relatively slow, since it involves the recalculation of the *complete* function for different values of $\varphi_{\mathbf{h}}$. Fortunately, the parameter-shift procedure will not be necessary for maximizing the Ω function, since a modified tangent formula (hereafter called the Ω tangent formula) can easily be derived.

By rearranging the terms of (16), the Ω function becomes

$$\begin{aligned} \Omega(\mathbf{t}) &= (1/3) \sum_{\mathbf{h}} \sum_{\mathbf{h}'} |E_{-\mathbf{h}} E_{\mathbf{h}'} E_{\mathbf{h}-\mathbf{h}'}| [W_{-\mathbf{h}} \cos(\Phi_3 + \xi_{-\mathbf{h}}) \\ &\quad + W_{\mathbf{h}'} \cos(\Phi_3 + \xi_{\mathbf{h}'}) + W_{\mathbf{h}-\mathbf{h}'} \cos(\Phi_3 + \xi_{\mathbf{h}-\mathbf{h}'})] \quad (18) \end{aligned}$$

$$= \sum_{\mathbf{h}} \sum_{\mathbf{h}'} v(\mathbf{h}, \mathbf{h}') |E_{-\mathbf{h}} E_{\mathbf{h}'} E_{\mathbf{h}-\mathbf{h}'}| \cos[\Phi_3 + \psi(\mathbf{h}, \mathbf{h}')] \quad (19)$$

with

$$\tan \psi(\mathbf{h}, \mathbf{h}') = (S_{-\mathbf{h}} + S_{\mathbf{h}'} + S_{\mathbf{h}-\mathbf{h}'}) / (C_{-\mathbf{h}} + C_{\mathbf{h}'} + C_{\mathbf{h}-\mathbf{h}'}) \quad (20)$$

$$\begin{aligned} v(\mathbf{h}, \mathbf{h}') &= (1/3) [(S_{-\mathbf{h}} + S_{\mathbf{h}'} + S_{\mathbf{h}-\mathbf{h}'})^2 \\ &\quad + (C_{-\mathbf{h}} + C_{\mathbf{h}'} + C_{\mathbf{h}-\mathbf{h}'})^2]^{1/2} \quad (21) \end{aligned}$$

$$C_{\mathbf{h}} = W_{\mathbf{h}} \cos \xi_{\mathbf{h}}, \quad S_{\mathbf{h}} = W_{\mathbf{h}} \sin \xi_{\mathbf{h}}. \quad (22), (23)$$

The derivation of the Ω tangent formula from (19) can be performed in a similar way to that in which Debaerdemaeker *et al.* (1985) derived the conventional tangent formula (Karle & Hauptman, 1956) from (1). Effectively, it may be assumed that a maximum of Ω corresponds to the true phase angles $\varphi_{\mathbf{h}}$. The condition for an extremum is then

$$\partial \Omega(\mathbf{t}) / \partial \varphi_{\mathbf{h}} = 0 \quad (24)$$

for every \mathbf{h} , so that

$$-2|E_{-\mathbf{h}}| \sum_{\mathbf{h}'} v(\mathbf{h}, \mathbf{h}') |E_{\mathbf{h}'} E_{\mathbf{h}-\mathbf{h}'}| \sin[\Phi_3 + \psi(\mathbf{h}, \mathbf{h}')] = 0. \quad (25)$$

Table 3. Some of the crystal structures used as a test for the Ω function

Code name	Molecular formula	Space group	Z	Reference
MBH2	C ₁₅ H ₂₄ O ₃	P1	3	(a)
NEWQB	C ₂₄ H ₂₀ N ₂ O ₅	P1̄ (as P1)	4	(b)
MUNICH1	C ₂₀ H ₁₆	C2	8	(c)
NO55	C ₂₀ H ₂₄ N ₄	Fdd2	16	(d)
TUR10	C ₁₅ H ₂₄ O ₂	P6 ₃ 22	12	(e)
BSS	C ₆ H ₁₈ B ₁₀ OS ₂	P2 ₁ /a (as P2 ₁)	4	(f)

References: (a) Poyser, Edwards, Anderson, Hursthouse, Walker, Sheldrick & Walley (1986); (b) Grigg, Kemp, Sheldrick & Trotter (1978); (c) Szeimies-Seebach, Harnisch, Szeimies, Van Meerssche, Germain & Declercq (1978); (d) Sheldrick & Trotter (1978); (e) Braekman, Daloze, Dupont, Tursch, Declercq, Germain & Van Meerssche (1981); (f) Rius, Miravittles, Viñas, Teixidor & Casabo (1989).

Table 4. Maximization of the Ω function with the Ω tangent formula

The 180 starting phases were computed with a five-atom fragment of MBH2 (9% scattering power).

Number of cycle	$ \Delta\varphi _{\max}$ (°)	Ω value
1	177	2102
2	47	2523
3	37	2592
4	22	2617
5	19	2632
6	53	2648
7	107	2683
8	26	2727
9	12	2749
10	6	2757
11	5	2760
12	4	2762
13	4	2763
14	3	2763
15	3	2763
16	2	2764

After some algebraic manipulation, (25) may be rearranged to give

$$\tan \varphi_{\mathbf{h}} = \left\{ \sum_{\mathbf{h}'} v(\mathbf{h}, \mathbf{h}') |E_{\mathbf{h}'} E_{\mathbf{h}-\mathbf{h}'}| \times \sin [\varphi_{\mathbf{h}'} + \varphi_{\mathbf{h}-\mathbf{h}'} + \psi(\mathbf{h}, \mathbf{h}')] \right\} \times \left\{ \sum_{\mathbf{h}'} v(\mathbf{h}, \mathbf{h}') |E_{\mathbf{h}'} E_{\mathbf{h}-\mathbf{h}'}| \times \cos [\varphi_{\mathbf{h}'} + \varphi_{\mathbf{h}-\mathbf{h}'} + \psi(\mathbf{h}, \mathbf{h}')] \right\}^{-1}. \quad (26)$$

The Ω tangent formula differs from the conventional one in the inclusion of the factor $v(\mathbf{h}, \mathbf{h}')$ and the phase shift $\psi(\mathbf{h}, \mathbf{h}')$. For illustrative purposes, the $v(\mathbf{h}, \mathbf{h}')$ and $\psi(\mathbf{h}, \mathbf{h}')$ values for the one-dimensional structure described in § 2.3. are given in Table 2.

3.3. Test calculations

Six test structures (Table 3) have been selected to illustrate the behaviour of the Ω function. The shift t in all the test calculations is $t = (t/c)\mathbf{c}$, where the shift length t ranges between 0.4 and 0.55 Å.

To prove the convergence of the Ω tangent formula, a series of phase refinements with starting phases computed from fragments of different size of MBH2

Table 5. Results of the application of the Ω tangent formula to the refinement of random phases

The maximum number of refinement cycles per trial is between 20 and 30.

Code	Number of reflections	Number of triplets	$\langle \alpha_{\text{est}} \rangle$	% of correct trials
MUNICH1	200	4986	22	2
NEWQB	250	2691	17	2
NO55	150	5844	25	1.5-2
TUR10	150	12174	39	12.5
BSS	150	4254	98	>15

were performed. The 180 reflections used were those with the largest E values ($\langle \alpha_{\text{est}} \rangle = 17$) and no rejection criterion was employed. Table 4 shows the refinement process of the phases computed with a five-atom fragment (9% scattering power). A weighted F_o synthesis computed with the first 52 peaks of the E map showed all the 54 atoms of the three independent molecules. Finally, an additional attempt to refine the phases from a four-atom fragment failed.

The Ω tangent formula can also be used for refining random starting phases, and its application to three structures that could not be solved by conventional direct methods (MUNICH1, NEWQB and NO55) and two easier ones (TUR10, BSS) has been investigated. The principal results are summarized in Table 5. A refined phase set is regarded as correct in Table 5 if a weighted F_o synthesis computed with the higher-ranked peaks of the E map reveals all the atoms of the structure. The number of higher-ranked peaks introduced is the number of atoms sought.

The results given in Table 5 are quite satisfactory and seem to indicate that, as predicted by the theory, the Ω tangent formula can be applied not only to low-symmetry space groups, but also to high-symmetry ones. On the other hand, the success rate is variable and, as is logical, seems to depend on the degree of difficulty of each particular structure, but, in any case, it is rather high. Moreover, the refinement of a large number of phase sets is not a problem, since the maximization of the Ω function with the Ω tangent formula is extremely fast.

It may be concluded that the Ω tangent formula is a useful tool for solving crystal structures. However, more practical experience is still necessary for optimizing its use.

Most calculations were performed with the OMEGA computer program (Rius & Miravittles, 1988). The weighted F_o syntheses and the peak interpretation were done with MULTAN84 (Main, Germain & Woolfson, 1984).

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References

- BAGGIO, R., WOOLFSON, M. M., DECLERCQ, J.-P. & GERMAIN, G. (1978). *Acta Cryst.* **A34**, 883-892.
- BHUIYA, A. K. & STANLEY, E. (1963). *Acta Cryst.* **16**, 981-984.
- BRAEKMAN, J. C., DALOZE, D., DUPONT, A., TURSCH, B., DECLERCQ, J.-P., GERMAIN, G. & VAN MEERSSCHE, M. (1981). *Tetrahedron*, **37**, 179-186.
- COCHRAN, W. (1952). *Acta Cryst.* **5**, 65-67.
- DEBAERDEMAEKER, T. (1982). Habilitationsschr. Univ. Ulm, Federal Republic of Germany.
- DEBAERDEMAEKER, T., TATE, C. & WOOLFSON, M. M. (1985). *Acta Cryst.* **A41**, 286-290.
- DEBAERDEMAEKER, T., TATE, C. & WOOLFSON, M. M. (1988). *Acta Cryst.* **A44**, 353-357.
- DEBAERDEMAEKER, T. & WOOLFSON, M. M. (1983). *Acta Cryst.* **A39**, 193-196.
- GRIGG, R., KEMP, J., SHELDRIK, G. & TROTTER, J. (1978). *J. Chem. Soc. Chem. Commun.* pp. 1109-1111.
- KARLE, J. & HAUPTMAN, H. (1956). *Acta Cryst.* **9**, 635-651.
- MAIN, P., GERMAIN, G. & WOOLFSON, M. M. (1984). *MULTAN84. A Computer Program for the Automatic Solution of Crystal Structures from X-ray Diffraction Data*. Univ. of York, England.
- POYSER, J. P., EDWARDS, R., ANDERSON, J., HURSTHOUSE, M., WALKER, N., SHELDRIK, G. & WALLEY, A. (1986). *J. Antibiot.* **39**, 167-169.
- RIUS, J. & MIRAVITLLES, C. (1988). *OMEGA88. A Computer Program for Solving Crystal Structures Based on the Omega Function*. CSIC, Inst. de Ciencia de Materials de Barcelona, Spain.
- RIUS, J., MIRAVITLLES, C., VIÑAS, C., TEIXIDOR, F. & CASABO, J. (1989). *Inorg. Chem.* Submitted.
- SAYRE, D. (1952). *Acta Cryst.* **5**, 60-65.
- SHELDRIK, G. & TROTTER, J. (1978). *Acta Cryst.* **B34**, 3122-3124.
- SZEIMIES-SEEBACH, U., HARNISCH, J., SZEIMIES, G., VAN MEERSSCHE, M., GERMAIN, G. & DECLERCQ, J.-P. (1978). *Angew. Chem. Int. Ed. Engl.* **17**, 848-850.
- YAO JIA-XING (1981). *Acta Cryst.* **A37**, 642-644.

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Definition of Symmetry Elements in Space Groups and Point Groups
Report of the International Union of Crystallography Ad-Hoc Committee on the
Nomenclature of Symmetry*

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Abstract

A 'geometric element' is defined, for any given symmetry operation, as a *geometric item that allows the operation (after removing any intrinsic translation) to be located and oriented*. In the case of an inversion, a (screw-) rotation or a (glide-) reflection, it is respec-

tively a point, line or plane. In the case of a rotoinversion, the geometric element consists of the axis of the rotation part and the center of the inversion part. As a general concept, the geometric element may be justified by a mathematical definition (as given in the Appendix). A 'symmetry element' (of a given crystal structure or object) is defined as a concept with a double meaning, namely *the combination of a geometric element with the set of symmetry operations having this geometric element in common ('element set')*. There is no overlap between element sets of a given structure. Together with the identity and the translations, for which a geometric element is not defined, the element sets cover all symmetry operations.

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