Conclusions

In the case of an orthorhombic crystal, the first and second partial derivatives of the lattice energy with respect to the cell parameters can be calculated by expressions like (16), where the repulsive coefficients b_{rs} and some of the charges z_r are considered as unknown parameters. By substituting the results into (8) and (9) a set of nine equations is obtained, which can be solved to determine up to nine wanted parameters.

A computer program (in Fortran IV) has been written to perform the calculations of the lattice-energy derivatives, using formulas (16)–(28): the computing scheme follows that of *MADEWA*, a program which calculates the electrostatic term of the lattice energy by Ewald series (Catti, 1978). The method developed here has been applied to forsterite, Mg_2SiO_4, assuming as unknown parameters in the lattice-energy expression three repulsive coefficients plus the electric charge on the oxygen atom (Catti, 1981); the overdetermined system of nine equations has been solved by a numeric procedure of minimization of the sum of squared deviations. The convergence rates of the series (17)–(28) have proved to be comparable with those of the corresponding integral series $F(\mathbf{x})$; as for the derivatives of the Ewald double sum, satisfactory results have been obtained using the same values of the parameter A which optimize the convergence of the Ewald series itself.

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Calculation of Even Moments of the Trigonometric Structure Factor. Methods and Results

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Abstract

Two algorithms for the evaluation of even moments of the trigonometric structure factor are described. The first algorithm is based on conventional structure-factor algebra in the complex notation and is applicable to any space group with multiplicity of general positions not exceeding 24. The second algorithm, capable of dealing with all space groups, involves an interpretation of trigonometrical expressions input in a symbolic form and a programmed execution of algebraic and analytic operations. The results obtained in this study include the fourth and sixth moments of the trigonometric structure factor for all 230 space groups. It is assumed that all the atoms occupy general positions. All the subsets of *hkl* indices giving rise to different forms of the trigonometric structure factor (except those for zones and rows) are considered.

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Introduction

Probability density functions of the structure amplitude $|F|$, which depend explicitly on the space-group symmetry and on the atomic composition of the asymmetric unit, were given by Karle & Hauptman (1953) and by Hauptman & Karle (1953) for centrosymmetric and non-centrosymmetric crystals respectively. Possible applications of these functions, which are asymptotic expansions in terms of the Wilson (1949) limiting distributions, to direct methods of phase determination have been discussed (Bertaut, 1955; Klug, 1958) and their application to intensity statistics investigated (Shmueli, 1979; Shmueli & Wilson, 1981). An obstacle that hindered an extensive application of these asymptotic expansions was, until recently, the necessity of obtaining the moments of the trigonometric structure factor for each space group considered. These moments are required for the evaluation of the symmetry-dependent parts of the expansion coefficients: for the nth expansion term, all the moments of the trigonometric structure factor, up to and including the $2n$th moment, are required.

The fourth moment of the trigonometric structure factor was evaluated (Wilson, 1978) for all the space groups but two, $Fd3m$ and $Fd3c$. This development enables one to evaluate the second term of either of the above asymptotic expansions. The need for the third term, and hence the sixth moment, arose in a recent study of intensity statistics (Shmueli & Wilson, 1981). It soon became clear that hand computations of this quantity for a wide range of space groups are forbiddingly tedious and it was therefore deemed worthwhile to construct computer-oriented algorithms which will render such computations rapid and insensitive to human error.

The purpose of this note is to present a description of these algorithms and to summarize the results obtained by their application to all the space groups.

These algorithms were already applied to all the symmorphic space groups with P-type Bravais lattices and the results for the fourth and sixth moments, for these space groups, are listed by Shmueli & Wilson (1981).

Description of the algorithms

Our application of conventional structure-factor algebra, in the complex notation, to the computation of even moments of the trigonometric structure factor, will be illustrated below by the calculation of the fourth moment.

The structure factor is given by

$$F(\mathbf{h}) = \sum_n f_n J_n(\mathbf{h}), \qquad (1)$$

where f_n is the scattering factor of atom n, $J_n(\mathbf{h})$ is its trigonometric structure factor and the summation ranges over all the atoms that comprise the asymmetric unit. The expression for $J_n(\mathbf{h})$ is

$$J_n(\mathbf{h}) = \sum_s \exp[2\pi i \mathbf{h}^T(\mathbf{P}_s \mathbf{r}_n + \mathbf{t}_s)], \qquad (2)$$

where $\mathbf{r}_n$ is the position vector of atom n, located in a Wyckoff position with multiplicity p_n, $\mathbf{h}^T = (hkl)$ is the diffraction vector and $(\mathbf{P}_s|\mathbf{t}_s)$ is a space-group operation. The summation in (2) ranges over all the space-group operations transforming $\mathbf{r}_n$ to its symmetry-equivalent positions in the unit cell. In what follows, only the case of general Wyckoff positions will be dealt with and the subscript n will therefore be omitted.

The average of $|J|^4$ taken over a large set of hkl values, or the fourth moment of $|J|$, can be written as

$$\langle |J|^4 \rangle = \langle (JJ^*)^2 \rangle = \sum_s \sum_t \sum_u \sum_v \langle \exp i(\varphi_{stuv} + \theta_{stuv}) \rangle, \qquad (3)$$

where

$$\varphi_{stuv} = 2\pi \mathbf{h}^T(\mathbf{P}_s - \mathbf{P}_t + \mathbf{P}_u - \mathbf{P}_v)\mathbf{r}$$

and

$$\theta_{stuv} = 2\pi \mathbf{h}^T(\mathbf{t}_s - \mathbf{t}_t + \mathbf{t}_u - \mathbf{t}_v).$$

If all the components of $\mathbf{r}$ do not happen to be simple fractions, φ_{stuv} can be assumed to be uniformly distributed over the $[0,2\pi]$ range. The above does not hold for θ_{stuv} and hence $\exp(i\theta_{stuv})$, or $\cos(\theta_{stuv})$ since $\langle |J|^4 \rangle$ is real, must be evaluated explicitly for each subset of hkl values that may be of interest. The average of a term in (3) is thus given by

$$\cos\theta_{stuv} \langle \exp(i\varphi_{stuv}) \rangle = \cos\theta_{stuv} \frac{1}{2\pi} \int_0^{2\pi} \exp(i\varphi)\, \mathrm{d}\varphi$$

$$= \begin{cases} \cos(\theta_{stuv}), & \text{for } \varphi_{stuv} \equiv 0 \\ 0 \quad , & \text{for } \varphi_{stuv} \not\equiv 0. \end{cases} \qquad (4)$$

Under the above circumstances, the necessary and sufficient condition for φ_{stuv} to be identically zero is that $\mathbf{P}_s - \mathbf{P}_t + \mathbf{P}_u - \mathbf{P}_v$ be a zero matrix. The same condition applies to a term in the summation for any even moment of $|J|$, the only difference being in the number of rotation matrices which have to be combined in the expression for φ.

For symmorphic space groups, *i.e.* in the absence of non-zero space-group translations, $\cos(\theta_{stuv})$ is unity throughout the summation and the fourth moment of $|J|$ may be obtained by simply counting the terms in (3) with zero matrices, rather than by algebraic and analytic manipulations of the relevant trigonometric expressions.

It therefore follows that any even moment of $|J|$ for these space groups must of necessity be an integer. As pointed out by Wilson (1978) this fact is not evident from calculations involving an averaging of even powers of trigonometric functions which appear in the corresponding expansions of $|J|^4$. Wilson (1978) showed, by considerations involving the Patterson function, that the fourth moment of $|J|$ must indeed be an integer, while the above result applies to any even moment.

For non-symmorphic space groups, the translation-dependent $\cos(\theta_{stuv})$ term may have to be evaluated separately for those subsets of hkl values which give rise to different functional forms of the real and imaginary parts of J (A and B in *International Tables*

Table 1. *The first three even moments of the trigonometric structure factor*

The symbols p, q and r denote the second, fourth and sixth moments of $|J|$. The ratios q/p^2 and r/p^3 are given as integers, exact decimal fractions or periodic decimal fractions. A dot above a digit indicates that this digit recurs indefinitely; *e.g.* $16{\cdot}319\dot{4} = 16{\cdot}31944\ldots = 16\frac{23}{72}$ In all cases, the result can be transformed to a simple fraction and the integers q and r recalculated.

Symmetry	p	q/p^2	r/p^3	Remarks‡
Point group: 1				
$P1$	1	1	1	
Point group: $\bar{1}$				
$P\bar{1}$	2	1·5	2·5	
Point groups: 2, m				
All P	2	1·5	2·5	
All C	4	3	10	
Point group: $2/m$				
All P	4	2.25	6·25	
All C	8	4·5	25	
Point group: 222				
All P	4	1·75	4	
All C and I	8	3·5	16	
$F222$	16	7	64	
Point group: $mm2$				
All P	4	2·25	6·25	
All A, C and I	8	4·5	25	
$Fmm2$	16	9	100	
$Fdd2$	16	9	100	(1)
	16	5	28	(2)
Point group: mmm				
All P	8	3·375	15·625	
All C and I	16	6·75	62·5	
$Fmmm$	32	13·5	250	
$Fddd$	32	13·5	250	(1)
	32	7.5	70	(2)
Point group: 4				
$P4$, $P4_2$	4	2·25	6·25	
$P4_1$*	4	2·25	6·25	(3)
	4	1·25	1·75	(4)
$I4$	8	4·5	25	
$I4_1$	8	4·5	25	(5)
	8	2·5	7	(6)
Point group: $\bar{4}$				
$P\bar{4}$	4	1·75	4	
$I\bar{4}$	8	3·5	16	
Point group: $4/m$				
All P	8	3·375	15·625	
$I4/m$	16	6·75	62·5	
$I4_1/a$†	16	6·75	62·5	(7)
	16	3·75	17·5	(8)
Point group: 422				
$P422$, $P42_12$, $P4_222$ and $P4_22_12$	8	2·125	6·625	
$P4_122$,* $P4_12_12$*	8	2·125	6·625	(3)
	8	1·625	3·25	(4)
$I422$	16	4·25	26·5	
$I4_122$	16	4·25	26·5	(7)
	16	3·25	13	(8)
Point group: $4mm$				
All P	8	2·625	10	
$I4mm$, $I4cm$	16	5·25	40	
$I4_1md$, $I4_1cd$	16	5·25	40	(7)
	16	3·25	13	(8)
Point groups: $\bar{4}2m$, $\bar{4}m2$				
All P	8	2·125	6·625	
$I\bar{4}2m$, $I\bar{4}m2$, $I\bar{4}c2$	16	4·25	26·5	
$I\bar{4}2d$	16	4·25	26·5	(5)
	16	3·25	13	(6)

Symmetry	p	q/p^2	r/p^3	Remarks‡
Point group: $4/mmm$				
All P	16	3·9375	25	
$I4/mmm$, $I4/mcm$	32	7·875	100	
$I4_1/amd$, $I4_1/acd$	32	7·875	100	(5)
	32	4·875	32·5	(6)
Point group: 3				
All P and R	3	$1{\cdot}\dot{6}$	$3{\cdot}\dot{4}$	
Point group: $\bar{3}$				
All P and R	6	2·5	$8{\cdot}6\dot{1}$	
Point group: 32				
All P and R	6	$1{\cdot}8\dot{3}$	$4{\cdot}6\dot{1}$	
Point group: $3m$				
$P3m1$, $P31m$, $R3m$	6	$1{\cdot}8\dot{3}$	$4{\cdot}9\dot{4}$	
$P3c1$, $P31c$, $R3c$	6	$1{\cdot}8\dot{3}$	$4{\cdot}9\dot{4}$	(3) (P), (1) (R)
	6	$1{\cdot}8\dot{3}$	$4{\cdot}2\dot{7}$	(4) (P), (2) (R)
Point group: $\bar{3}m$				
$P\bar{3}1m$, $P\bar{3}m1$, $R\bar{3}m$	12	2·75	$12{\cdot}36\dot{1}$	
$P\bar{3}1c$, $P\bar{3}c1$, $R\bar{3}c$	12	2·75	$12{\cdot}36\dot{1}$	(3) (P), (1) (R)
	12	2·75	$10{\cdot}69\dot{4}$	(4) (P), (2) (R)
Point group: 6				
$P6$	6	2·5	$9{\cdot}\dot{4}$	
$P6_1$*	6	2·5	$9{\cdot}\dot{4}$	(9)
	6	1·5	$2{\cdot}52\dot{7}$	(10)
	6	1·5	$2{\cdot}69\dot{4}$	(11)
	6	2·5	$7{\cdot}\dot{7}$	(12)
$P6_2$*	6	2·5	$9{\cdot}\dot{4}$	(13)
	6	1·5	$2{\cdot}69\dot{4}$	(14)
$P6_3$	6	2·5	$9{\cdot}\dot{4}$	(3)
	6	2·5	$7{\cdot}\dot{7}$	(4)
Point group: $\bar{6}$				
$P\bar{6}$	6	2·5	$8{\cdot}6\dot{1}$	
Point group: $6/m$				
$P6/m$	12	3·75	$23{\cdot}6\dot{1}$	
$P6_3/m$	12	3·75	$23{\cdot}6\dot{1}$	(3)
	12	3·75	$19{\cdot}\dot{4}$	(4)
Point group: 622				
$P622$	12	2·25	$7{\cdot}986\dot{1}$	
$P6_122$*	12	2·25	$7{\cdot}986\dot{1}$	(9)
	12	1·75	$4{\cdot}0069\dot{4}$	(10)
	12	1·75	$4{\cdot}0486\dot{1}$	(11)
	12	2·25	$7{\cdot}569\dot{4}$	(12)
$P6_222$*	12	2·25	$7{\cdot}986\dot{1}$	(13)
	12	1·75	$4{\cdot}0486\dot{1}$	(14)
$P6_322$	12	2·25	$7{\cdot}986\dot{1}$	(3)
	12	2·25	$7{\cdot}569\dot{4}$	(4)
Point group: $6mm$				
$P6mm$	12	2·75	$13{\cdot}402\dot{7}$	
$P6cc$	12	2·75	$13{\cdot}402\dot{7}$	(3)
	12	2·75	$10{\cdot}069\dot{4}$	(4)
$P6_3cm$, $P6_3mc$	12	2·75	$13{\cdot}402\dot{7}$	(3)
	12	2·75	$11{\cdot}319\dot{4}$	(4)
Point group: $\bar{6}m2$, $\bar{6}2m$				
$P\bar{6}m2$, $P\bar{6}2m$	12	2·75	$12{\cdot}36\dot{1}$	
$P\bar{6}c2$, $P\bar{6}2c$	12	2·75	$12{\cdot}36\dot{1}$	(3)
	12	2·75	$10{\cdot}69\dot{4}$	(4)
Point group: $6/mmm$				
$P6/mmm$	24	4·125	$33{\cdot}5069\dot{4}$	
$P6/mcc$	24	4·125	$33{\cdot}5069\dot{4}$	(3)
	24	4·125	$25{\cdot}1736\dot{1}$	(4)
$P6_3/mcm$, $P6_3/mmc$	24	4·125	$33{\cdot}5069\dot{4}$	(3)
	24	4·125	$28{\cdot}2986\dot{1}$	(4)

Table 1 (*cont.*)

Symmetry	p	q/p^2	r/p^3	Remarks‡
Point group: 23				
$P23$, $P2_13$	12	$1\cdot91\dot{6}$	$5\cdot2\dot{7}$	
$I23$, $I2_13$	24	$3\cdot8\dot{3}$	$21\cdot\dot{1}$	
$F23$	48	$7\cdot\dot{6}$	$84\cdot\dot{4}$	
Point group: $m3$				
$Pm3$, $Pn3$, $Pa3$	24	$3\cdot125$	$16\cdot319\dot{4}$	
$Im3$, $Ia3$	48	$6\cdot25$	$65\cdot2\dot{7}$	
$Fm3$	96	$12\cdot5$	$261\cdot\dot{1}$	
$Fd3$	96	$12\cdot5$	$261\cdot\dot{1}$	(1)
	96	$10\cdot5$	$161\cdot\dot{1}$	(2)
Point group: 432				
$P432$, $P4_232$	24	$2\cdot208\dot{3}$	$8\cdot069\dot{4}$	
$P4_132$*†	24	$2\cdot208\dot{3}$	$8\cdot069\dot{4}$	(15)
	24	$2\cdot041\dot{6}$	$6\cdot19\dot{4}$	(16)
	24	$1\cdot8750$	$4\cdot819\dot{4}$	(17)
	24	$1\cdot708\dot{3}$	$3\cdot9\dot{4}$	(18)
$I432$	48	$4\cdot41\dot{6}$	$32\cdot2\dot{7}$	
$I4_132$†	48	$4\cdot41\dot{6}$	$32\cdot2\dot{7}$	(15)
	48	$3\cdot75$	$19\cdot2\dot{7}$	(19)
$F432$	96	$8\cdot8\dot{3}$	$129\cdot\dot{1}$	
$F4_132$	96	$8\cdot8\dot{3}$	$129\cdot\dot{1}$	(15)
	96	$6\cdot8\dot{3}$	$63\cdot\dot{1}$	(18)

Symmetry	p	q/p^2	r/p^3	Remarks‡
Point group: $\bar{4}3m$				
$P\bar{4}3m$	24	$2\cdot208\dot{3}$	$8\cdot902\dot{7}$	
$P\bar{4}3n$	24	$2\cdot208\dot{3}$	$8\cdot902\dot{7}$	(1)
	24	$2\cdot208\dot{3}$	$7\cdot236\dot{1}$	(2)
$I\bar{4}3m$	48	$4\cdot41\dot{6}$	$35\cdot6\dot{1}$	
$I\bar{4}3d$†	48	$4\cdot41\dot{6}$	$35\cdot6\dot{1}$	(15); (20)
	48	$4\cdot41\dot{6}$	$28\cdot9\dot{4}$	(15); (21)
	48	$3\cdot75$	$19\cdot2\dot{7}$	(19)
$F\bar{4}3m$	96	$8\cdot8\dot{3}$	$142\cdot\dot{4}$	
$F\bar{4}3c$	96	$8\cdot8\dot{3}$	$142\cdot\dot{4}$	(15)
	96	$8\cdot8\dot{3}$	$115\cdot\dot{7}$	(18)
Point group: $m3m$				
$Pm3m$, $Pn3m$	48	$3\cdot8125$	$31\cdot319\dot{4}$	
$Pn3n$, $Pm3n$	48	$3\cdot8125$	$31\cdot319\dot{4}$	(1)
	48	$3\cdot8125$	$24\cdot652\dot{7}$	(2)
$Im3m$	96	$7\cdot625$	$125\cdot2\dot{7}$	
$Ia3d$†	96	$7\cdot625$	$125\cdot2\dot{7}$	(15); (20)
	96	$7\cdot625$	$98\cdot6\dot{1}$	(15); (21)
	96	$5\cdot625$	$46\cdot9\dot{4}$	(19)
$Fm3m$	192	$15\cdot25$	$501\cdot\dot{1}$	
$Fm3c$	192	$15\cdot25$	$501\cdot\dot{1}$	(1)
	192	$15\cdot25$	$394\cdot\dot{4}$	(2)
$Fd3m$	192	$15\cdot25$	$501\cdot\dot{1}$	(1)
	192	$11\cdot25$	$211\cdot\dot{1}$	(2)
$Fd3c$	192	$15\cdot25$	$501\cdot\dot{1}$	(1)
	192	$11\cdot25$	$184\cdot\dot{4}$	(2)

* And the enantiomorphous space group.

† One or more q values for this space group are inconsistent with those given by Wilson (1978) (see text).

‡ Remarks: (1) $h+k+l=2n$; (2) $h+k+l=2n+1$; (3) $l=2n$; (4) $l=2n+1$; (5) $2h+l=2n$; (6) $2h+l=2n+1$; (7) $2k+l=2n$; (8) $2k+l=2n+1$; (9) $l=6n$; (10) $l=6n+1, 6n+5$; (11) $l=6n+2, 6n+4$; (12) $l=6n+3$; (13) $l=3n$; (14) $l=3n+1$; $3n+2$; (15) hkl all even; (16) only one index odd; (17) only one index even; (18) hkl all odd; (19) two indices odd; (20) $h+k+l=4n$; (21) $h+k+l=4n+2$.

for X-ray Crystallography, 1952) within the same space group. The procedure of computing $\langle |J|^4\rangle$ for a given subset of hkl is first to locate a term in (3) for which φ_{stuv} is zero and then to accumulate the corresponding value of $\cos(\theta_{stuv})$. Such a contribution may, in general, have one of the values: 0, $\pm\frac{1}{2}$, ±1, depending on the denominators of the fractional translations present. The fact that the fourth moment of $|J|$ is invariably an integer is due to the inherent symmetry of the summation (3).

An extension of the above method to the calculation of any even moment of $|J|$ is self-evident.

The above method was successfully applied to the evaluation of the fourth and sixth moments of $|J|$ for a large number of space groups, with the multiplicity of general Wyckoff positions not exceeding 24. For higher multiplicities the method was found to be too slow, mainly for the sixth moment, on which most of the computing time is spent. Thus, the moments $\langle |J|^4\rangle$ and $\langle |J|^6\rangle$ for $P6/mmm$ ($p=24$) required about $2\frac{1}{2}$ min computing time on a CDC6600 and the corresponding moments for $Pm3m$ ($p=48$) would call for about ten times as much, the symmetry of the sixfold summation being allowed for. Some usual programming shortcuts, such as packing rotation matrices into single words and preliminary storage of difference matrices, were used.

In the second algorithm, developed for the more extensive calculations, the expressions for A and B, taken directly from *International Tables for X-ray Crystallography* (1952), are employed. These expressions are, if necessary, transformed to sums of triple sine/cosine products. Each triple product is input in a symbolic form (*e.g.* $\cos 2\pi kx \cos 2\pi hy \sin 2\pi lz$ is read in as CKXCHYSLZ) which is decoded by the program. The required powers of the trigonometric polynomials are then evaluated, the terms containing odd powers of sines and/or cosines are deleted and the remaining ones are averaged by appropriate substitutions of the integral

$$\frac{1}{2\pi}\int_0^{2\pi}\sin^{2m}x\cos^{2n}x\,\mathrm{d}x=\frac{(2m-1)!!(2n-1)!!}{(2m+2n)!!},\qquad m,n>0,\tag{5}$$

where $(2k-1)!!=1.3\ldots(2k-1)$ and $(2k)!!=$

$2^k k!$, with the understanding that for, say, $m = 0$ (5) reduces to $(2n-1)!!/(2n)!!$

The above procedure can readily cope with the calculation of $\langle |J|^4 \rangle$ and $\langle |J|^6 \rangle$ for any space group. This symbol-handling procedure is also much faster than the first one. Thus, the values of $\langle |J|^4 \rangle$ and $\langle |J|^6 \rangle$ for the cubic system, the most complex one, including separate calculations for the various *hkl* subsets, have been obtained in less than $1\frac{1}{2}$ min on a CDC6600. However, when the trigonometrical forms given for A and B need extensive rearrangements (*e.g.* for trigonal and hexagonal systems), the structure-factor algebraic procedure described above is preferable in practice.

Results

The fourth and sixth moments of the trigonometric structure factor were computed for all 230 space groups and the results are summarized in Table 1.

Since the symmetry-dependent coefficients required for the evaluation of moments and distributions of the normalized structure factor depend on the ratios q/p^2 and r/p^3, where $p = \langle |J|^2 \rangle$, $q = \langle |J|^4 \rangle$, $r = \langle |J|^6 \rangle$ (Shmueli & Wilson, 1981), and these ratios, rather than the individual moments, are likely to be of use, the results are presented in their terms. Of course, q and r can be readily found since p is given for each entry.

It was assumed throughout the calculation that all the atoms occupy general positions and all the subsets of *hkl* (except those corresponding to zones and rows), giving rise to different functional forms of A and B, were considered. The absence of any remark beside an entry in Table 1 means that all the space groups and/or all the above mentioned subsets of *hkl* corresponding to this entry lead to identical values of p, q and r.

In the comparison of our results for q with those obtained by Wilson (1978) it is appropriate to point out that his results were obtained without the aid of a computer and that the possibility of his tables containing some errors was emphasized (*cf.* §1.7; Wilson, 1978). The comparison showed a single numerical discrepancy ($I4_1/a$), one inconsistent association of a q value with an *hkl* subset ($P4_132$) and two more q values for $P4_132$ not given by Wilson (1978). Also Wilson's values of q for $I4_132$, $I\bar{4}3d$ and $Ia3d$, unlike the other entries in his Table 3 (Wilson, 1978), are not the average q values but coincide with ours for the '*hkl* all even' case. For all the rest, there is an exact agreement regarding q values for primitive space groups and average q values for the centered ones. The values of q for the space groups $Fd3m$ and $Fd3c$, not given by Wilson (1978), were supplied in this work.

Corresponding results for the eighth moment of $|J|$ can now also be computed and will be reported later.

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Stacking Faults and Twins in Kyanite, Al_2SiO_5

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Abstract

Two types of twins are frequently found in naturally and experimentally deformed kyanite. Structural models based on periodic shears are proposed to account for these mechanical twins. The structure of kyanite is then regarded as layered, the limits of each layer being easy glide planes for dislocations. The shear plane is (100). The shear vectors are $\frac{1}{2}$ [001] and $\frac{1}{2}$ [011]. They are suitable for the only known glide system (100) [001].

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