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Structure Factor and Least-Squares Calculation for Orthorhombic Systems with Anisotropic Vibrations*

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A set of expressions is presented for calculating structure factors and least-squares coefficients for orthorhombic structures containing atoms with anisotropic temperature factors. These expressions are analogous to those previously derived by Rollett and Davies (1955) for monoclinic space groups.

Introduction

The increased availability of high-speed digital computers for crystallographic calculations has made practical more accurate determinations of atomic parameters with the inclusion of anisotropic thermal vibrations of the atoms in the analysis. This increase in computer utilization has been paralleled by an increase in the use of the least-squares method (Hughes, 1941) for the refinement of the various parameters. Three features make the least-squares method particularly suitable for machine computation. First, any desired weighting function may be prescribed. Second, totals for the normal equations can be accumulated in concurrence with the calculation of the structure factors. Third, the procedure is iterative.

The programming of digital computers for structure factors and least-squares calculations has followed two courses. The first course makes use of no lattice symmetry; by using redundant parameters and calculating symmetry equivalent reflections one can obtain results consistent with any space group (Sparks, Prosen, Kruse, & Trueblood, 1956). Proponents of this method consider the ease of coding to justify the computing inefficiency encountered in symmetric structures. Following the other course are those who program the computer for specific crystal classes (see, for example, Lavine & Rollett, 1956), feeling that the saving of computing time warrants the additional efforts invested in programming.

With this latter course in mind, Rollett & Davies (1955), hereafter RD, have derived a set of expressions that can be used to calculate structure factors and least-squares coefficients for any monoclinic space group. It is the purpose of the present paper to present an analogous, though somewhat more complicated, set of expressions that are applicable to all orthorhombic symmetries.In developing these expressions we make use of the formulations of Trueblood (1956) and the International Tables (1952).

General (*hkl*) structure factor

We shall start with the expression for the scattering factor for a vibrating atom:

$$f_1 = f_0 \exp -(B_{11}h^2 + B_{22}k^2 + B_{33}l^2 + B_{12}hk + B_{13}hl + B_{23}kl) ,$$

where f_0 is the scattering factor for the atom at rest. As explained by RD, the orthorhombic symmetry gives rise, in general, to three additional orientations of the vibrational ellipsoid; and we write the corresponding scattering factors:

$$f_2 = f_0 \exp -(B_{11}h^2 + B_{22}k^2 + B_{33}l^2 + B_{12}hk - B_{13}hl - B_{23}kl)$$

$$f_3 = f_0 \exp -(B_{11}h^2 + B_{22}k^2 + B_{33}l^2 - B_{12}hk + B_{13}hl - B_{23}kl)$$

$$f_4 = f_0 \exp -(B_{11}h^2 + B_{22}k^2 + B_{33}l^2 - B_{12}hk - B_{13}hl + B_{23}kl)$$

RD also showed that the structure factor expression for any orthorhombic space group contains the term $(f_1+f_2+f_3+f_4)$ and three terms in which two of f_2, f_3 and f_4 are negative. Accordingly we define, in

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Table 1. *Scattering factor combinations and their derivatives*

Definitions	$\partial E/\partial B_{11}$	$\partial E/\partial B_{22}$	$\partial E/\partial B_{33}$	$\partial E/\partial B_{12}$	$\partial E/\partial B_{13}$	$\partial E/\partial B_{23}$	$\partial E/\partial B$
$f_1+f_2+f_3+f_4=E_1$	E_1	E_1	E_1	E_2	E_3	E_4	E_1
$f_1+f_2-f_3-f_4=E_2$	E_2	E_2	E_2	E_1	E_4	E_3	0
$f_1-f_2+f_3-f_4=E_3$	E_3	E_3	E_3	E_4	E_1	E_2	0
$f_1-f_2-f_3+f_4=E_4$	E_4	E_4	E_4	E_3	E_2	E_1	0
Multiplicative constants obtained from the differentiation	$-h^2$	$-k^2$	$-l^2$	$-hk$	$-hl$	$-kl$	$-\sin^2\theta/\lambda^2$

Table 1, the four functions E_1, E_2, E_3 and E_4 and their derivatives with respect to the temperature coefficients. (For the isotropic case, where $f_1=f_2=f_3=f_4=f_0 \exp(-B \sin^2\theta/\lambda^2)$, $E_1=4f_1$ and $E_2=E_3=E_4=0$). We see that each derivative is, except for a multiplicative constant, equal to one of the E's.

We next introduce the trigonometric portions of the scattering factors. There are eight possible combinations of triple products of sines and cosines, which we call T_1–T_8; these, together with their products, P, with the various E's, are defined in Table 2. The resulting P's are now combined in eight different ways (see Table 3) to form the pertinent coefficients S_1–S_8. With the exception of certain classes of reflections in space groups *Fdd2* and *Fddd*, the structure factor and all the parameter derivatives for any reflection in the orthorhombic system contain as the principal factor one or another of these S's.

The cascade of definitions culminates in Table 4, which, in conjunction with Tables 5 and 6, provides the prescription for choosing the S functions appropriate to any class of reflections in any orthorhombic space group.

We now introduce the relations $|F|^2=\varrho_c^2(A^2+B^2)$, $\partial|F|^2/\partial\xi=2\varrho_c^2(A\partial A/\partial\xi+B\partial B/\partial\xi)$ and $A=\sum_i \varrho_i A_i$, $B=\sum_i \varrho_i B_i$. Here ϱ_c reflects the space-group multiplicity. For acentric primitive space groups ϱ_c has the value unity; a center of symmetry introduces a factor of two, the non-primitive lattices A, C and I contribute a factor of two, while a face-centered lattice F, a factor of four. We also introduce ϱ_i as a population parameter which, if other than unity, indicates either partial occupancy of an atomic site or an atom in a special position having multiplicity less than that of the space group. By including ϱ_i in the least-squares treatment, one can obtain information concerning either the over-all scale factor or the degree of occupancy of the site.

We suggest that when using these tables one start by finding the appropriate space group listing in Table 5. From there one obtains the value of ϱ_c, the type designation and the group key as a function of the index parity tests. The lefthand column of Table 4 contains the constant that multiplies both parts (A and B) of the relation whose A term is listed under 'Functions'. The value of A_i and the derivatives of A with respect to the various positional and temperature-factor parameters ($\partial A/\partial\xi$) can then be selected according to which of the four groups the particular reflection falls into. The terms involving B, however, require that we first separate the space groups into the three crystal classes 222–D_2 (denoted Type I in Table 4 and 5), *mm2*–C_{2v} (Type II), and *mmm*–D_{2h} (Type III). The last two columns of Table 4 provide the key for choosing the correct functions of B for space groups of Type I and II; since those of Type III are centrosymmetric, no B term is necessary (provided the origin of coordinates is chosen at the center of symmetry, as is customary).

Table 2. *Trigonometric combinations and their products with the scattering factors*

Definition	Product with E_1	E_2	E_3	E_4
$\cos 2\pi hx.\cos 2\pi ky.\cos 2\pi lz = T_1$	P_1	P_9	P_{17}	P_{25}
$\cos 2\pi hx.\cos 2\pi ky.\sin 2\pi lz = T_2$	P_2	P_{10}	P_{18}	P_{26}
$\cos 2\pi hx.\sin 2\pi ky.\cos 2\pi lz = T_3$	P_3	P_{11}	P_{19}	P_{27}
$\cos 2\pi hx.\sin 2\pi ky.\sin 2\pi lz = T_4$	P_4	P_{12}	P_{20}	P_{28}
$\sin 2\pi hx.\cos 2\pi ky.\cos 2\pi lz = T_5$	P_5	P_{13}	P_{21}	P_{29}
$\sin 2\pi hx.\cos 2\pi ky.\sin 2\pi lz = T_6$	P_6	P_{14}	P_{22}	P_{30}
$\sin 2\pi hx.\sin 2\pi ky.\cos 2\pi lz = T_7$	P_7	P_{15}	P_{23}	P_{31}
$\sin 2\pi hx.\sin 2\pi ky.\sin 2\pi lz = T_8$	P_8	P_{16}	P_{24}	P_{32}

Table 3. *The eight pertinent terms.*

$S_1=P_1-P_{15}-P_{22}-P_{28}$	$S_5=P_5+P_{11}+P_{18}-P_{32}$
$S_2=P_2-P_{16}+P_{21}+P_{27}$	$S_6=P_6+P_{12}-P_{17}+P_{31}$
$S_3=P_3+P_{13}-P_{24}+P_{26}$	$S_7=P_7-P_9+P_{20}+P_{30}$
$S_4=P_4+P_{14}+P_{23}-P_{25}$	$S_8=P_8-P_{10}-P_{19}-P_{29}$

Table 4. *The prescription for obtaining structure factor and derivative terms for any orthorhombic space group.*

Multiplicative constants	Functions	Group* 1	2	3	4	Type I	Type II
1	A_i	$+S_1$	$-S_4$	$-S_7$	$-S_6$	—	$\partial B/\partial z$
$2\pi\varrho_i h$	$\partial A/\partial x$	$-S_5$	$+S_8$	$-S_3$	$-S_2$	$-\partial B/\partial B_{23}$	$-\partial B/\partial B_{13}$
$2\pi\varrho_i k$	$\partial A/\partial y$	$-S_3$	$-S_2$	$-S_5$	$+S_8$	$-\partial B/\partial B_{13}$	$-\partial B/\partial B_{23}$
$2\pi\varrho_i l$	$\partial A/\partial z$	$-S_2$	$-S_3$	$+S_8$	$-S_5$	$-\partial B/\partial B_{12}$	$-B_i$
$-hk\varrho_i$	$\partial A/\partial B_{12}$	$-S_7$	$-S_6$	$+S_1$	$-S_4$	$\partial B/\partial z$	—
$-hl\,\varrho_i$	$\partial A/\partial B_{13}$	$-S_6$	$-S_7$	$-S_4$	$+S_1$	$\partial B/\partial y$	$\partial B/\partial x$
$-kl\,\varrho_i$	$\partial A/\partial B_{23}$	$-S_4$	$+S_1$	$-S_6$	$-S_7$	$\partial B/\partial x$	$\partial B/\partial y$
1	—	$+S_8$	$-S_5$	$-S_2$	$-S_3$	$-B_i$	$-\partial B/\partial B_{12}$
$-h^2\varrho_i$	$\partial A/\partial B_{11}$	Same as for A_i and B_i					
$-k^2\varrho_i$	$\partial A/\partial B_{22}$	Same as for A_i and B_i					
$-l^2\,\varrho_i$	$\partial A/\partial B_{33}$	Same as for A_i and B_i					
$-\varrho_i \sin^2\theta/\lambda^2$	$\partial A/\partial B$	Same as for A_i and B_i					
1	$\partial A/\partial\varrho_i$	Same as for A_i and B_i					

* V_i or W_i replace S_i whenever specified by Table 5. Type III: The imaginary parts of the expressions are all zero.

Table 5. *A tabulation of the orthorhombic space groups according to class and index parities*

Space group	Class: Type	Class: ϱ_c	Planes	Group key
$P222$	I	1	All planes	1
$P222_1$	I	1	l even	1
			l odd	2
$P2_12_12$	I	1	$(h+k)$ even	1
			$(h+k)$ odd	3
$P2_12_12_1$	I	1	$(h+k)$ even, $(k+l)$ even	1
			$(h+k)$ even, $(k+l)$ odd	2
			$(h+k)$ odd, $(k+l)$ odd	3
			$(h+k)$ odd, $(k+l)$ even	4
$C222_1$	I	2	$(h+k)$ even, l even	1
			$(h+k)$ even, l odd	2
$C222$	I	2	$(h+k)$ even	1
$F222$	I	4	$(h+k)$ even and $(k+l)$ even	1
$I222$	I	2	$(h+k+l)$ even	1
$I2_12_12_1$	I	2	h even and k even and l even	1
			h even and k odd and l odd	4
			h odd and k even and l odd	3
			h odd and k odd and l even	2
$Pmm2$	II	1	All planes	1
$Pmc2_1$	II	1	l even	1
			l odd	2
$Pcc2$	II	1	l even	1
			l odd	3
$Pma2$	II	1	h even	1
			h odd	3
$Pca2_1$	II	1	h even and l even	1
			h even and l odd	4
			h odd and l even	3
			h odd and l odd	2
$Pnc2$	II	1	$(k+l)$ even	1
			$(k+l)$ odd	3
$Pmn2_1$	II	1	$(h+l)$ even	1
			$(h+l)$ odd	2
$Pba2$	II	1	$(h+k)$ even	1
			$(h+k)$ odd	3
$Pna2_1$	II	1	$(h+k)$ even and l even	1
			$(h+k)$ even and l odd	4
			$(h+k)$ odd and l even	3
			$(h+k)$ odd and l odd	2
$Pnn2$	II	1	$(h+k+l)$ even	1
			$(h+k+l)$ odd	3
$Cmm2$	II	2	$(h+k)$ even	1
$Cmc2_1$	II	2	$(h+k)$ even and l even	1
			$(h+k)$ even and l odd	2
$Ccc2$	II	2	$(h+k)$ even and l even	1
			$(h+k)$ even and l odd	3
$Amm2$	II	2	$(k+l)$ even	1
$Abm2$	II	2	$(k+l)$ even, k even	1
			$(k+l)$ even, k odd	3
$Ama2$	II	2	$(k+l)$ even, and h even	1
			$(k+l)$ even, and h odd	3
$Aba2$	II	2	$(k+l)$ even, $(h+k)$ even	1
			$(k+l)$ even, $(h+k)$ odd	3
$Fmm2$	II	4	$(h+k)$ even, $(k+l)$ even	1

Table 5 (*cont.*)

Space group	Class: Type	Class: ϱ_c		Group key
Fdd2	II	4	$h+k+l=4n$, $(h+l)$ even, $(k+l)$ even	1
			$h+k+l=4n+1$, $(h+l)$ even, $(k+l)$ even	1*
			$h+k+l=4n+2$, $(h+l)$ even, $(k+l)$ even	3
			$h+k+l=4n+3$, $(h+l)$ even, $(k+l)$ even	3*
Imm2	II	2	$(h+k+l)$ even	1
Iba2	II	2	$(h+k+l)$ even and l even	1
			$(h+k+l)$ even and l odd	3
Iam2	II	2	$(h+k+l)$ even and h even	1
			$(h+k+l)$ even and h odd	3
Pmmm	III	2	All planes	1
Pnnn	III	2	$(h+k)$ even and $(k+l)$ even	1
			$(h+k)$ even and $(k+l)$ odd	3
			$(h+k)$ odd and $(k+l)$ even	2
			$(h+k)$ odd and $(k+l)$ odd	4
Pccm	III	2	l even	1
			l odd	3
Pbam	III	2	h even and k even	1
			h even and k odd	4
			h odd and k even	2
			h odd and k odd	3
Pmma	III	2	h even	1
			h odd	4
Pnna	III	2	h even and $(k+l)$ even	1
			h even and $(k+l)$ odd	3
			h odd and $(k+l)$ even	2
			h odd and $(k+l)$ odd	4
Pmna	III	2	$(h+l)$ even	1
			$(h+l)$ odd	2
Pcca	III	2	h even and l even	1
			h even and l odd	3
			h odd and l even	4
			h odd and l odd	2
Pbam	III	2	$(h+k)$ even	1
			$(h+k)$ odd	3
Pccn	III	2	$(h+k)$ even and $(h+l)$ even	1
			$(h+k)$ even and $(h+l)$ odd	3
			$(h+k)$ odd and $(h+l)$ even	2
			$(h+k)$ odd and $(h+l)$ odd	4
Pbcm	III	2	k even and l even	1
			k even and l odd	2
			k odd and l even	3
			k odd and l odd	4
Pnnm	III	2	$(h+k+l)$ even	1
			$(h+k+l)$ odd	3
Pmmn	III	2	h even and k even	1
			h even and k odd	2
			h odd and k even	4
			h odd and k odd	3
Pbcn	III	2	$(h+k)$ even and l even	1
			$(h+k)$ even and l odd	2
			$(h+k)$ odd and l even	4
			$(h+k)$ odd and l odd	3
Pbca	III	2	$(h+k)$ even and $(k+l)$ even	1
			$(h+k)$ even and $(k+l)$ odd	2
			$(h+k)$ odd and $(k+l)$ even	4
			$(h+k)$ odd and $(k+l)$ odd	3
Pnma	III	2	$(h+l)$ even and k even	1
			$(h+l)$ even and k odd	3
			$(h+l)$ odd and k even	4
			$(h+l)$ odd and k odd	2

Table 5 (*cont.*)

Space group	Class: Type	Class: ϱ_c	Planes	Group key
Cmcm	III	4	$(h+k)$ even and l even	1
			$(h+k)$ even and l odd	2
Cmca	III	4	$(h+k)$ even and $(k+l)$ even	1
			$(h+k)$ even and $(k+l)$ odd	2
Cmmm	III	4	$(h+k)$ even	1
Cccm	III	4	$(h+k)$ even and l even	1
			$(h+k)$ even and l odd	3
Cmma	III	4	$(h+k)$ even and h even	1
			$(h+k)$ even and h odd	2
Ccca	III	4	$(h+k)$ even and k even and l even	1
			$(h+k)$ even and k even and l odd	3
			$(h+k)$ even and k odd and l even	4
			$(h+k)$ even and k odd and l odd	2
Fmmm	III	8	$(h+k)$ even and $(k+l)$ even	1
Fddd	III	8	$h+k=4n$, $l+h=4n$, $k+l=4n$	1
			$h+k=4n$, $l+h=4n+2$, $k+l=4n+2$	3
			$h+k=4n+2$, $l+h=4n+2$, $k+l=4n$	2
			$h+k=4n+2$, $l+h=4n$, $k+l=4n+2$	4
			$h+k=4n$, $l+h=4n+2$, $k+l=4n$	1†
			$h+k=4n$, $l+h=4n$, $k+l=4n+2$	3†
			$h+k=4n+2$, $l+h=4n$, $k+l=4n$	2†
			$h+k=4n+2$, $l+h=4n+2$, $k+l=4n+2$	4†
Immm	III	4	$(h+k+l)$ even	1
Ibam	III	4	$(h+k+l)$ even, l even	1
			$(h+k+l)$ even, l odd	3
Ibca	III	4	$(h+k+l)$ even, h even, k even	1
			$(h+k+l)$ even, h even, k odd	4
			$(h+k+l)$ even, h odd, k even	3
			$(h+k+l)$ even, h odd, k odd	2
Imma	III	4	$(h+k+l)$ even, k even	1
			$(h+k+l)$ even, k odd	2

* Use V_{1-8} in place of S_{1-8}. † Use W_{1-8} in place of S_{1-8}.

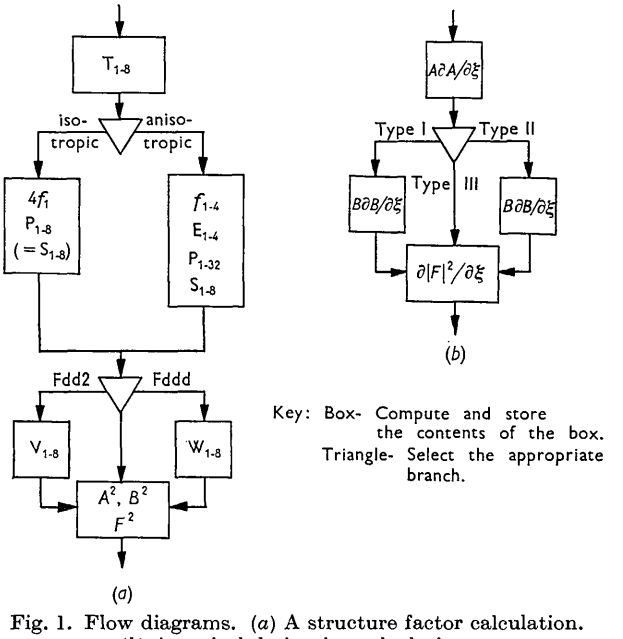
Table 6. *The special terms required for space groups Fdd2 and Fddd*

$V_1=0{\cdot}5\ \ (S_1-S_2-S_7-S_8)$	$W_1=0{\cdot}5\ \ (S_1-S_4+S_6-S_7)$
$V_2=0{\cdot}5\ \ (S_1+S_2+S_7-S_8)$	$W_2=0{\cdot}5\ \ (S_2+S_3-S_5-S_8)$
$V_3=0{\cdot}5\ \ (S_3-S_4+S_5+S_6)$	$W_3=0{\cdot}5\ \ (S_2+S_3+S_5+S_8)$
$V_4=0{\cdot}5\ \ (S_3+S_4-S_5+S_6)$	$W_4=0{\cdot}5(-S_1+S_4+S_6-S_7)$
$V_5=0{\cdot}5\ \ (S_3+S_4+S_5-S_6)$	$W_5=0{\cdot}5(-S_2+S_3+S_5-S_8)$
$V_6=0{\cdot}5(-S_3+S_4+S_5+S_6)$	$W_6=0{\cdot}5\ \ (S_1+S_4+S_6+S_7)$
$V_7=0{\cdot}5(-S_1-S_2+S_7-S_8)$	$W_7=0{\cdot}5(-S_1-S_4+S_6+S_7)$
$V_8=0{\cdot}5\ \ (S_1-S_2+S_7+S_8)$	$W_8=0{\cdot}5(-S_2-S_3-S_5-S_8)$

Application

As an example illustrating the use of Table 4 and 5, let us consider the reflections with k and l odd in space group $Abm2$–C_{2v}^{15}. From Table 5 we find that this space group is Type II and the reflections are in group 3; accordingly $A_i=(-S_7)_i$, $B_i=-(+S_8)_i$, and $(\partial|F|^2/\partial B_{13})_i=-2(2^2)hl\varrho_i\{A(-S_4)_i+B[-(-S_3)_i]\}$.

Certain classes of reflections in space groups *Fdd2* and *Fddd* require separate treatment. For them it is convenient to use additional functions V_{1-8} or W_{1-8}, as defined in Table 6, which are substituted for the



Key: Box- Compute and store the contents of the box.
Triangle- Select the appropriate branch.

Fig. 1. Flow diagrams. (*a*) A structure factor calculation. (*b*) A typical derivative calculation.

corresponding S functions and used as prescribed in Table 4.

A suggested procedure for calculating structure factors and derivatives is illustrated in Fig. 1. For each atom i, the trigonometric triple products $(T_{1-8})_i$ are first calculated. The intermediate products $(P_{1-32})_i$ are then formed, and these are combined to give the coefficients $(S_{1-8})_i$. (For an isotropic atom, only P_{1-8} need be calculated since $P_{1-8}=S_{1-8}$). Space group and index parity tests are then made, and if necessary the additional functions $(V_{1-8})_i$ or $(W_{1-8})_i$ are calculated. The correct structure factor and derivative terms are then selected in accordance with Table 4.

We have used these orthorhombic expressions and also the monoclinic expressions of RD as the bases for two separate structure factor and least-squares programs for the Burroughs 220 computer. This computer has an access time of approximately 100 microseconds; a complete structure factor least-squares calculation, including the collecting of 7×7 matrices involving scale and temperature-factor derivatives for each atom, takes approximately 0·25 seconds per atom reflection. Isotropic atoms, for which many of the calculations can be by-passed, require less than half this time.

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Least Squares Refinement of the Structure of Gadolinium-Iron Garnet, $Gd_3Fe_2Fe_3O_{12}$

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X-ray diffraction photographs of gadolinium–iron garnet, $Gd_3Fe_2Fe_3O_{12}$, show Laue symmetry $m3m$, and systematic extinctions indicate $Ia3d$ as the most probable space group. There are eight formula weights per unit cell with $a=12{\cdot}470\pm0{\cdot}005$ Å. Positions of all ions except O^{2-} are fixed by the space group. The least-squares method has been applied to refine the oxygen coordinates, using only 75 structure factors with significant oxygen contributions. The final values obtained for the coordinates are $x=-0{\cdot}0269$, $y=0{\cdot}0550$, and $z=0{\cdot}1478$. Interionic distances and angles calculated from these coordinates are nearly identical to the corresponding distances and angles in yttrium–iron garnet, as predicted by magnetic data.

Difficulties were encountered in the least-squares refinement of the structure. The use of limited numbers of structure factor data gave rise to large interactions between the temperature factors of the metal ions. A separate refinement with additional data was necessary to evaluate these thermal parameters.

Introduction

Gadolinium–iron garnet is one of a series of ferrimagnetic oxides of general formula $R_3Fe_2Fe_3O_{12}$, where R represents yttrium or a rare-earth element with $Z=62$ to 71 inclusive. Bertaut & Forrat (1956) and Geller & Gilleo (1957*a*) have shown that these synthetic garnets have the same crystal structure as that of the natural garnets, which was established by Menzer (1928) from X-ray powder photographs. Similar compounds with aluminium or gallium replacing iron have also been prepared (Yoder & Keith, 1951; Keith & Roy, 1954). The first detailed X-ray single crystal work on the synthetic garnets has been carried out by Geller & Gilleo (1957*b*, 1959), who have refined the structure of yttrium–iron garnet. Because detailed information is of importance in understanding magnetic properties, it appears desirable to carry out structure analyses for other garnets to determine the effects of cation substitution upon the crystal structure.

The unknown parameters in the garnet structure are the oxygen–ion coordinates, the oxygen–ion temperature factor, and the temperature factors of the