to E values of about 1·4 contributes only limited configurational information. Expansion to E values of 1·0 adds no new information and, due to the squaring effect, may even destroy valuable phase information. The use of the different phase expansion procedure, 'phase correction', eliminates the squaring tendency and allows phase expansion to E values of 1·0. Compared with the tangent formula the phases are more accurate resulting in a narrow range of atomic peak heights, few or no interspersed spurious peaks, elimination of wrong peaks, enhancement of unknown atoms and reduction of background. Phase sets treated with the tangent formula which do not converge to an interpretable or partially recognizable structure may be improved by phase correction to show the complete structure.

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Classification of Magnetic Structures in Some Orthorhombic Space Groups

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The magnetic structures belonging to magnetic space groups isomorphic with D_{2h}^i, $i=1,2,\ldots 16$, are classified for the general and special positions of these space groups.

Introduction

Given a crystal with ionic magnetic moments $\mathbf{S}_1$, $\mathbf{S}_2,\ldots,\mathbf{S}_n$ on a set of n-fold positions, the $3n$ dimensional space

$$\mathbf{S}=\mathbf{S}_1\times\mathbf{S}_2\times\ldots\mathbf{S}_n \qquad (1)$$

has subspaces invariant under the paramagnetic symmetry group of the crystal. The bases of all these subspaces, known as modes* (Bertaut, 1968), may serve to classify the possible magnetic structures in the crystal. A classification of this sort for special positions in D_{2h}^{16} is given in the literature (Bertaut, 1968). We present an extension of the classification to 2-, 4- and 8-fold positions in D_{2h}^i, $i=1,2,\ldots,16$, as a part of an idea to extend the classification to all space groups. Tables of limiting conditions for allowed reflexions in these space groups are given elswhere (Gurewitz & Shaked, 1971). An example of the use of the classification scheme and the tables of allowed reflexions in the analysis of neutron diffraction from a polycrystalline sample of $KFeCl_3$, is given in the present paper.

* In analogy with normal modes of the theory of vibrations.

Classification of the magnetic structures in crystals belonging to D_{2h}^i, $i=1,2,\ldots 16$

The point group of the space groups D_{2h}^i is *mmm*. This is a commutative group of order 8. It has: (*a*) seven

subgroups of order 4, three of type *mm*, one of type 222, and three of type $2/m$ (*b*) seven subgroups of order 2, three of type *m*, one of type $\bar{1}$, and three of type 2. The multiplicity of a position with a certain point symmetry equals the index of this point group with respect to *mmm*. Hence, the 2- or 4-fold special positions in D_{2h}^i have the point symmetry of one of the subgroups (*a*) or (*b*) respectively.

The irreducible representations of *mmm* are real and one-dimensional. It is therefore possible to decompose the space **S** [equation (1)] into $3n$ one-dimensional subspaces, invariant with respect to D_{2h}^i. Since an orthorhombic axis, $\alpha=x,y,z$, transforms into $\pm\alpha$ under *mmm* we could choose V_α^u as bases to the invariant subspaces of **S**, namely:

$$V_\alpha^u=\sum_{j=1}^{n}\lambda_{j\alpha}^u S_{j\alpha}\,, \tag{2}$$

where $\alpha=x,y,z$ and $u=1,2,\ldots,n$.

The irreducible representation of any element of *mmm* is either $+1$ or -1 and it follows* that

$$\lambda_{j\alpha}^u=+1,-1\,. \tag{3}$$

We may choose $\lambda_{1\alpha}^u=\lambda_1=+1$ for every u and α. In order to determine the values of the rest of the $\lambda_{j\alpha}^u$, we utilize the following property: for every symmetry element in D_{2h}^i, we can rewrite equation (2) in pairs, $\lambda_{l\alpha}^u S_{l\alpha}+\lambda_{k\alpha}^u S_{k\alpha}$, so that the magnetic moment in the position l transforms to a magnetic moment in the position k, and *vice versa*, under the transformation of this symmetry element. A necessary and sufficient condition that V_α^u be invariant under this symmetry element is that the products $\lambda_{l\alpha}^u\lambda_{k\alpha}^u$ are the same for all pairs in equation (2) of every symmetry element. This condition is independent of α and it is therefore convenient to look for the 'vector solutions':

$$\mathbf{V}^u=\sum\lambda_j^u\mathbf{S}_j\,. \tag{4}$$

Every one of the three components of $\mathbf{V}^u$ is an invariant subspace. Consider the factor group of *mmm* relative to the group of the point symmetry of an *n*-fold position. A generator, A_q, of this factor group transforms $\mathbf{S}_1$ to $\mathbf{S}_q$; hence, it forms the product $\lambda_1\lambda_q^u=\lambda_q^u$, which can take either $+1$ or -1. If we have w generators, there are 2^w solutions, which is just the index of the group of point symmetry relative to *mmm*. Hence, there are n 'vector solutions' [equation (4)] and $3n$ scalar solutions [equation (2)] as required to span the space **S** [equation (1)]. One 'vector solution' is all

Table 1. *Definition of the twofold position labels with respect to the symmetry element*

Point symmetry	Symmetry elements transforming position no. 1 to position no.: 1		2	
$2_\gamma/m_\gamma$	E	$\bar{1}$	m_α	m_β
	m_γ	2_γ	2_α	2_β
222	E	2_α	$\bar{1}$	m_α
	2_β	2_γ	m_β	m_γ
$m_\alpha m_\beta$	E	2_γ	$\bar{1}$	m_γ
	m_α	m_β	2_α	2_β

Table 2. *Definition of the fourfold position labels with respect to the symmetry elements*

Point symmetry	Symmetry elements transforming position no. 1 to position no.: 1		2		3		4	
m_α	E	m_α	$\bar{1}$	2_α	2_β	m_γ	2_γ	m_β
2_α	E	2_α	$\bar{1}$	m_α	m_β	m_γ	2_γ	2_β
$\bar{1}$	E	$\bar{1}$	m_y	2_y	m_x	2_x	m_z	2_z

Table 3. *Definition of the general position labels with respect to the symmetry elements*

Symmetry elements transforming position no. 1 to position no.: 1	2	3	4	5	6	7	8
E	2_y	2_x	2_z	$\bar{1}$	m_y	m_x	m_z

* The sum [equation (2)] can be obtained by operating with the projection operator on the vector $S_{1\alpha}$. $\lambda_{j\alpha}^u$ is the representation of the symmetry element which transforms the position 1 to the position *j*.

Table 4. *Magnetic groups and corresponding magnetic structures in the two-, four- and eight-fold positions in* D_{2h}^i, $i=1,2,\ldots,16$ (*Gurewitz & Shaked*, 1971)

(1)	Two fold									Four fold									Eight fold		
(2)	$2_\gamma/m_\gamma$			2_α 2_β 2_γ			$m_\alpha m_\beta$			m_α			2_α			$\bar{1}$			1	
(4) (3)	α	β	γ	α	β	γ	α	β	γ	α	β	γ	α	β	γ	α	β	γ	α	β	γ
m_α m_β m_γ	–	–	A	–	–	–	–	–	F	C	–	–	C	–	–	G	C	A	G^+	C^+	A^+
m_α m_β m_γ	–	–	F	–	–	F	–	–	F	–	C	F	–	C	F	C	G	F	C^+	G^+	F^+
m_α m_β m_γ	A	F	–	–	F	–	–	F	–	–	F	C	–	F	C	A	F	G	A^+	F^+	G^+
m_α m_β m_γ	F	A	–	F	–	–	F	–	–	F	–	–	F	–	–	F	A	C	F^+	A^+	C^+
m_α m_β m_γ	–	–	–	–	–	–	–	–	A	–	G	A	G	–	–	–	–	–	G^-	C^-	A^-
m_α m_β m_γ	–	–	–	–	–	A	–	–	–	G	–	–	–	G	A	–	–	–	C^-	G^-	F^-
m_α m_β m_γ	–	–	–	–	A	–	A	–	–	A	–	–	–	A	G	–	–	–	A^-	F^-	G^-
m_α m_β m_γ	–	–	–	A	–	–	–	A	–	–	A	G	A	–	–	–	–	–	F^-	A^-	C^-

(1) Multiplicity
(2) Point symmetry
(3) Magnetic axis parallel to:
(4) Magnetic group

$\lambda_j^1 = +1$ (ferromagnetic). In the other $n-1$ solutions, half of the λ's are $+1$ and half are -1 (antiferromagnetic). The 'vector solution', $\mathbf{V}^u$, is sometimes called magnetic configuration (Shirane, 1959), the name we use in the rest of the paper.

We now write down* the magnetic configurations for the $n=2$-, 4- and 8-fold positions in D_{2h}^l, $i=$

* We use the symbols **F, C, G, A** (Bertaut, 1968) rather than $\mathbf{V}^u$.

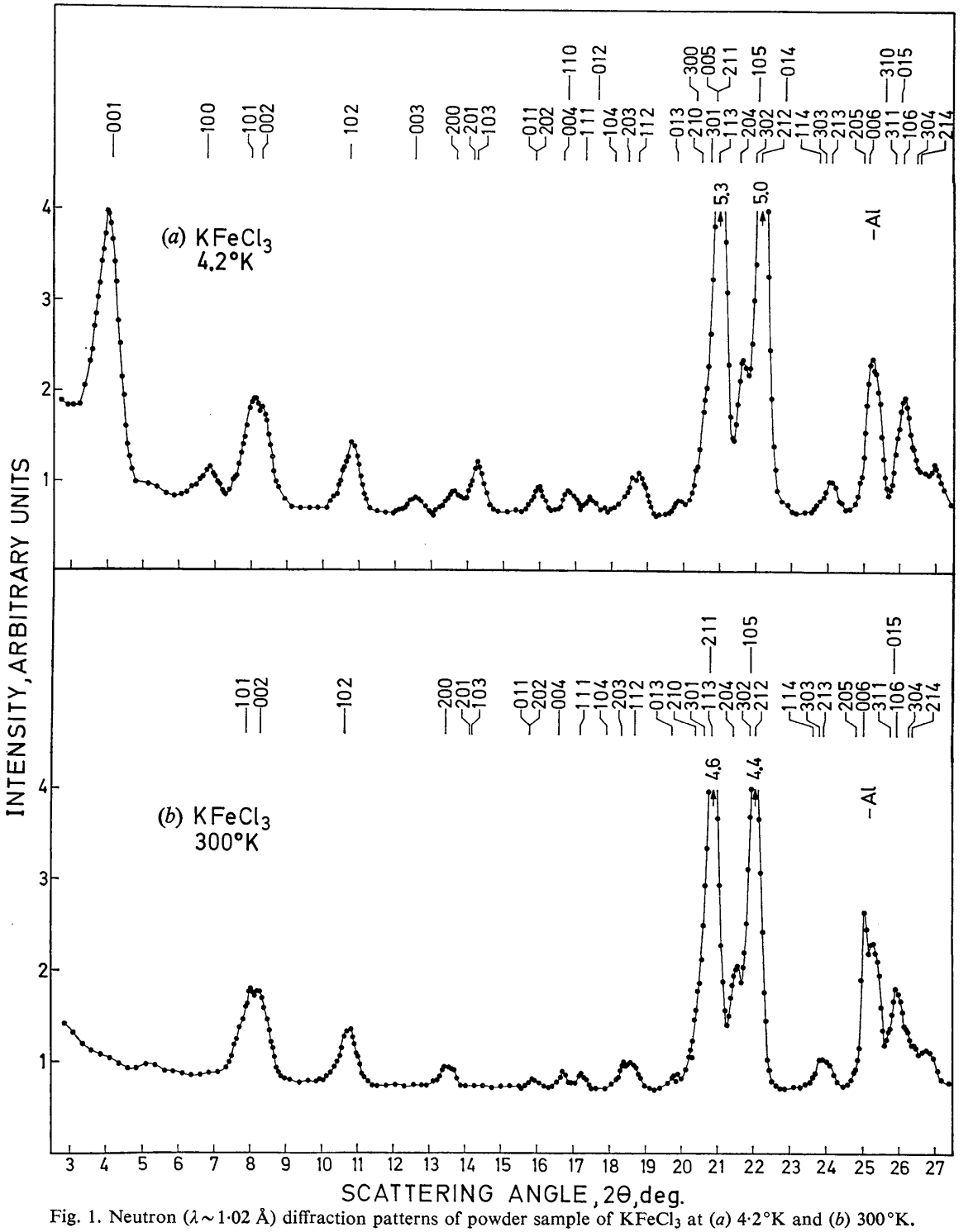

Fig. 1. Neutron ($\lambda \sim 1{\cdot}02$ Å) diffraction patterns of powder sample of $KFeCl_3$ at (*a*) 4·2°K and (*b*) 300°K.

1,2, . . . ,16. The correspondence between the position q and the symmetry element that transforms position 1 into position q is given in Tables 1, 2 and 3. Position 1 is any of the n positions.

A. The two ($n=2$) fold positions allow one ferromagnetic and one antiferromagnetic configuration:

$$\begin{aligned}\mathbf{F}&=\mathbf{S}_1+\mathbf{S}_2\\ \mathbf{A}&=\mathbf{S}_1-\mathbf{S}_2\,.\end{aligned}\qquad(5)$$

Table 5. *Limiting conditions on possible reflexions*

Special pos tions m, in D_{2h}^i, $i=1,2,\ldots 16$ (Gurewitz & Shaked, 1971).

SPACE GROUP	P. Symmetry	Wyckoff Nota.	LIMITING CONDITIONS hkℓ	F	C	A	G
Pmmm	m_x	u,v	00ℓ, h0ℓ	No Cond.	-	No Cond.	-
			0k0, hk0	No Cond.	-	-	No Cond.
			h00	No Cond.	-	-	-
	m_y	w,x	00ℓ, 0kℓ	No Cond.	-	-	No Cond.
			0k0	No Cond.	-	-	-
			h00, hk0	No Cond.	-	No Cond.	-
	m_z	y,z	00ℓ	No Cond.	-	-	-
			0k0, 0kℓ	No Cond.	-	No Cond.	-
			h00, h0ℓ	No Cond.	-	-	No Cond.
Pccm	m_z	q	00ℓ	ℓ=2n	ℓ=2n+1	-	-
			0k0	No Cond.	-	No Cond.	-
			0kℓ	ℓ=2n	ℓ=2n+1	ℓ=2n	ℓ=2n+1
			h00	No Cond.	-	-	No Cond.
			h0ℓ	ℓ=2n	ℓ=2n+1	ℓ=2n+1	ℓ=2n
Pmma	m_y	i,j	00ℓ, 0kℓ	No Cond.	-	-	No Cond.
			0k0	No Cond	-	-	-
			h00, hk0	h=2n	h=2n+1	h=2n	h=2n+1
	m_x	k	00ℓ, h0ℓ	No Cond.	-	No Cond.	-
			0k0	No Cond.	-	-	No Cond.
			hk0	h=2n	h=2n+1	h=2n+1	h=2n
			h00	h=2n	-	h=2n+1	-
Pmna	m_x	h	00ℓ	ℓ=2n	ℓ=2n+1	ℓ=2n	ℓ=2n+1
			0k0	No Cond.	-	-	No Cond.
			h00	h=2n	h=2n+1	-	-
			h0ℓ	h+ℓ=2n	h+ℓ=2n+1	h+ℓ=2n	h+ℓ=2n+1
			hk0	h=2n	h=2n+1	h=2n+1	h=2n
Pbam	m_z	g,h	00ℓ	No Cond.	-	-	-
			0k0, 0kℓ	k=2n	k=2n+1	k=2n	k=2n+1
			h00, h0ℓ	h=2n	h=2n+1	h=2n+1	h=2n
Pbcm	m_z	d	00ℓ	ℓ=2n	-	ℓ=2n+1	-
			0k0, 0kℓ	k=2n	k=2n+1	k=2n	k=2n+1
			h00	No Cond.	-	-	No Cond.
			h0ℓ	ℓ=2n	ℓ=2n+1	ℓ=2n+1	ℓ=2n
Pnnm	m_z	g	00ℓ	ℓ=2n	ℓ=2n+1	-	-
			0k0	k=2n	k=2n+1	k=2n	k=2n+1
			0kℓ	k+ℓ=2n	k+ℓ=2n+1	k+ℓ=2n	k+ℓ=2n+1
			h00	h=2n	h=2n+1	h=2n+1	h=2n
			h0ℓ	h+ℓ=2n	h+ℓ=2n+1	h+ℓ=2n+1	h+ℓ=2n
Pmmn	m_x	i	00ℓ, h0ℓ	No Cond.	-	No Cond.	-
			0k0	k=2n	k=2n+1	k=2n+1	k=2n
			h00	h=2n	-	h=2n+1	-
			hk0	h+k=2n	h+k=2n+1	h+k=2n+1	h+k=2n
	m_y	f	00ℓ, 0kℓ	No Cond.	-	-	No Cond.
			0k0	k=2n	-	-	k=2n+1
			h00	h=2n	h=2n+1	h=2n	h=2n+1
			hk0	h+k=2n	h+k=2n+1	h+k=2n	h+k=2n+1
Pnma	m_y	c	00ℓ	ℓ=2n	ℓ=2n+1	ℓ=2n+1	ℓ=2n
			0k0	k=2n	-	h=2n	-
			h00, hk0	h=2n	h=2n+1	h=2n	h=2n+1
			0kℓ	k+ℓ=2n	k+ℓ=2n+1	k+ℓ=2n+1	k+ℓ=2n

B. The four ($n=4$) fold positions allow one ferromagnetic and three antiferromagnetic configurations:

$$\begin{aligned}\mathbf{F}&=\mathbf{S}_1+\mathbf{S}_2+\mathbf{S}_3+\mathbf{S}_4\\ \mathbf{G}&=\mathbf{S}_1-\mathbf{S}_2+\mathbf{S}_3-\mathbf{S}_4\\ \mathbf{A}&=\mathbf{S}_1-\mathbf{S}_2-\mathbf{S}_3+\mathbf{S}_4\\ \mathbf{C}&=\mathbf{S}_1+\mathbf{S}_2-\mathbf{S}_3-\mathbf{S}_4\,.\end{aligned}\qquad(6)$$

C. The eight ($n=8$) fold positions allow one ferromagnetic and seven antiferromagnetic configurations:

$$\begin{aligned}\mathbf{F}^+&=\mathbf{S}_1+\mathbf{S}_2+\mathbf{S}_3+\mathbf{S}_4+\mathbf{S}_5+\mathbf{S}_6+\mathbf{S}_7+\mathbf{S}_8\\ \mathbf{G}^+&=\mathbf{S}_1-\mathbf{S}_2+\mathbf{S}_3-\mathbf{S}_4+\mathbf{S}_5-\mathbf{S}_6+\mathbf{S}_7-\mathbf{S}_8\\ \mathbf{A}^+&=\mathbf{S}_1-\mathbf{S}_2-\mathbf{S}_3+\mathbf{S}_4+\mathbf{S}_5-\mathbf{S}_6-\mathbf{S}_7+\mathbf{S}_8\\ \mathbf{C}^+&=\mathbf{S}_1+\mathbf{S}_2-\mathbf{S}_3-\mathbf{S}_4+\mathbf{S}_5+\mathbf{S}_6-\mathbf{S}_7-\mathbf{S}_8\\ \mathbf{F}^-&=\mathbf{S}_1+\mathbf{S}_2+\mathbf{S}_3+\mathbf{S}_4-\mathbf{S}_5-\mathbf{S}_6-\mathbf{S}_7-\mathbf{S}_8\\ \mathbf{G}^-&=\mathbf{S}_1-\mathbf{S}_2+\mathbf{S}_3-\mathbf{S}_4-\mathbf{S}_5+\mathbf{S}_6-\mathbf{S}_7+\mathbf{S}_8\\ \mathbf{A}^-&=\mathbf{S}_1-\mathbf{S}_2-\mathbf{S}_3+\mathbf{S}_4-\mathbf{S}_5+\mathbf{S}_6+\mathbf{S}_7-\mathbf{S}_8\\ \mathbf{C}^-&=\mathbf{S}_1+\mathbf{S}_2-\mathbf{S}_3-\mathbf{S}_4-\mathbf{S}_5-\mathbf{S}_6+\mathbf{S}_7+\mathbf{S}_8\,.\end{aligned}\qquad(7)$$

As already mentioned, the components of a configuration (say G_x, G_y, and G_z of **G**) represent three possible magnetic modes. The magnetic symmetries of the magnetic modes are summarized in Table 4. For example, consider a crystal of the space group *Pbcn* (D_{2h}^{14}) having magnetic ions at the 4(*c*) positions, the point symmetry of which is 2_y (*International Tables for X-ray Crystallography*, 1969). In using Table 4, we therefore set $\alpha\rightarrow y$, $\beta\rightarrow z$, $\gamma\rightarrow x$, and it follows that the mode C_y belongs to *Pbcn*, the modes C_z and F_x belong to *Pbc'n'*, and so on.

Example

The compound $KFeCl_3$ is orthorhombic with *Pnma* as a space group at room temperature (Gurewitz, Makovsky & Shaked, 1972). The magnetic Fe^{2+} ions are located at the 4(*c*) positions (point symmetry: m_y). This compound undergoes a para to antiferromagnetic transition at about 15 °K. Neutron diffraction patterns of a polycrystalline sample at 4·2 and 300 °K are shown in Fig. 1. Magnetic contributions [Fig. 1(*a*)] to the reflexions: {001}, {100}, {101}, {102}, {003}, {201}, {110}, {300} and {310} are observed. According to Table 5, the reflexions {00*l*} with $l=2n+1$ and {*h*00} with $h=2n+1$ are allowed only in the **C** configuration. Furthermore, these reflexions exclude (because of q^2) structures with $M\|z$ or $M\|x$. We can, therefore, conclude that the only axial structure consistent with the neutron data (Fig. 1) is **C** with $M\|y$, or C_y.* In order to determine the magnetic space group, we note that the point symmetry is m_y; therefore we set in Table 4

* It still remains to be shown that the integrated intensities calculated for C_y are in agreement with the observed ones.

the correspondence $m_y \leftrightarrow m_\alpha$, namely $\alpha \leftrightarrow y$. Hence, C_y appears in the first line (under m_α), and the magnetic group according to which C_y (C_α) transforms is (Table 4) *Pnma* ($m_\alpha m_\beta m_\gamma$).

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Properties of Crystal Lattices: The Derivative Lattices and their Determination

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Derivative lattices are classified as super, sub and composite, on the basis of the properties of the transformation matrices relating them to the lattice from which they are derived. A method for obtaining the transformation matrices generating these lattices is given. The method has been applied to the derivation of the unique super and sublattices in a few important cases.

The super and sublattices associated with the lattice of a crystal are not infrequently related to important properties of the crystal. For example, in the case of twinning by reticular merohedry, twinning takes place only if a superlattice possesses symmetry (or pseudosymmetry) higher than that of the crystal lattice (Friedel, 1964; Donnay, Donnay & Kullerud, 1958). The concepts of super and sublattices are also essential in the study of some derivative structures (Buerger, 1946, 1954). In an order–disorder transformation, for example, the ordered phase is characterized by a cell larger than that of the disordered phase and, similarly, the cell on which a magnetic structure is based is often larger than that of the corresponding chemical structure. So far, no attempt has been made to determine systematically the number and the geometrical properties of super and sublattices associated with a given lattice, and the treatment of this subject has been generally restricted to specific cases of interest. In this paper, we define derivative lattices and then outline a method for their derivation.

Let us consider any given lattice and let us describe it in terms of any arbitrary primitive triplet of noncoplanar translations $\mathbf{a}_i$ (a triplet is called *primitive* when it defines a primitive cell: *International Tables for X-ray Crystallography*, 1969, p. 8). Let us now perform the axial transformation

$$\mathbf{b}_i = \sum_j S_{ij}\mathbf{a}_j \quad (i,j=1,2,3) \qquad (1)$$

and let us assume that the determinant $|\mathbf{S}|$ of the transformation matrix $\mathbf{S}$ is different from zero. The three noncoplanar translations $\mathbf{b}_i$ can be regarded as the edges of a primitive cell defining a new lattice related to the one based on the translations $\mathbf{a}_i$ by transformation (1). We may call *original lattice* the lattice based on the triplet of translations $\mathbf{a}_i$ and *derivative lattice* the lattice defined by the triplet of translations $\mathbf{b}_i$, provided that this triplet is considered primitive. Original and derivative lattices are in general different, *i.e.* they have different reduced cells (Niggli, 1928; *International Tables for X-ray Crystallography*, 1969, p. 530). However, if the elements S_{ij} are integers, and if the determinant $|\mathbf{S}|$ is equal to unity, the two lattices are identical.

The derivative lattices of interest in crystallography are those that are obtained when the elements S_{ij} in transformation (1) are simple rational numbers. These lattices can be defined in terms of the properties of the transformation matrix $\mathbf{S}$ as follows.

Definition 1. A derivative lattice is a *superlattice*,* if the elements S_{ij} of matrix $\mathbf{S}$ are integers, and if the determinant $|\mathbf{S}|$ is greater than one. Thus, all the nodes of the superlattice are nodes of the original lattice, but not all nodes of the original lattice are nodes of the superlattice.

Definition 2. Let $\mathbf{T}$ be the inverse of matrix $\mathbf{S}$, *i.e.* $\mathbf{T}=\mathbf{S}^{-1}$. A derivative lattice is a *sublattice*, if the elements T_{ij} of matrix $\mathbf{T}$ are integers, and if the determinant $|\mathbf{T}|$ is greater than one. Thus all the nodes of

* In some publications, especially in the mathematical literature (*e.g.* Cassels, 1959), a 'superlattice' as defined in this paper is called a sublattice because it is generated by a subgroup of the translations on which the original lattice is based.