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Spin Translation Groups and Neutron Diffraction Analysis

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Groups that are a generalization of magnetic groups, and called 'spin groups', are defined. Among the spin groups those called 'spin translation groups' are tabulated and described in some detail. The possible magnetic reflexions of unpolarized neutrons elastically scattered from a single crystal whose spin arrangement is invariant under a spin translation group are also tabulated. It is shown how by using these tables and considering the indices of magnetic reflexions one can obtain information on the mutual orientation of non-collinear spins without making any assumptions on the rotational symmetry of the spin arrangement. As an example of this, the neutron diffraction data of the 'umbrella' spin arrangement of CrSe is reanalysed.

1. Introduction

Two group-theoretical methods have been applied in determining the spin arrangement of a magnetic crystal from neutron diffraction data. One is the method of Donnay, Corliss, Donnay, Elliott & Hastings (1958) based on the theory of magnetic groups, and the second the method of Bertaut (1968) based on the theory of the representations of space groups. Opechowski & Dreyfus (1971) have shown in which sense the two group-theoretical methods are equivalent.

In the method based on magnetic groups, spin arrangements are uniquely characterized by a label which contains in the simplest case the magnetic symmetry group of the spin arrangement and the orientation and magnitude of a single spin. For spin arrangements where the magnetic symmetry group is a two-dimensional magnetic space group one needs to specify in such a label an infinite number of spins. In the case of a helical spin arrangement whose magnetic symmetry group is two-dimensional it is sufficient to specify several or even only one spin together with a group of rotations (Opechowski & Dreyfus, 1971). Such additional symmetries are closely related to the generalized magnetic groups considered by Nash (1963) and Kitz (1965) and called 'spin-space' groups by Brinkman & Elliott (1965). We will call such groups simply 'spin' groups. One can from the outset characterize spin arrangements using these spin groups instead of magnetic groups.

In this paper we give a precise definition of spin groups and consider in detail a subclass of these groups named spin translation groups. In § 2 we review the transformation properties of a spin arrangement upon the application of space-group and magnetic-group elements and discuss the concept of spin-group elements. Spin translation are defined in § 3 and the possible magnetic reflexions of unpolarized neutrons elastically scattered from a single crystal whose spin arrangement is invariant under a spin translation group are derived in § 4. In § 5 we apply the theory of spin translation groups to the analysis of neutron diffraction data and show how information on the mutual orientation of non-collinear spins can be obtained without making any assumptions on the rotational symmetry of the spin arrangement. We then consider as an example the analysis of neutron diffraction data from powdered chronium selenide.

2. Spin symmetry

A spin arrangement, in the purely geometric point of view adopted in this paper, means an axial vector function denoted by $\mathbf{S}(\mathbf{r})$ that changes sign under time inversion, defined on a set of points (atoms) which form a crystal. We will call the vectors 'spins' and the vector space to which these spins belong the 'spin space'.

The usual notation of a space group element G is $(R|\mathbf{v})$ where R is a proper or improper rotation matrix and $\mathbf{v}$ is a column matrix representing a primitive or non-primitive translation. Applying G to a spin arrangement $\mathbf{S}(\mathbf{r})$ means replacing $\mathbf{S}(\mathbf{r})$ by the spin arrangement which we denote by $[R\|R|\mathbf{v}]\mathbf{S}(\mathbf{r})$ and is defined in Opechowski & Guccione (1965) by

$$[R\|R|\mathbf{v}]S^i(\mathbf{r}) = \sum_{j=1}^{3} \delta_R R_{ij} S^j((R|\mathbf{v})^{-1}\mathbf{r}) \qquad (1)$$

where $\delta_R = \det R$ and $i = 1,2,3$. As apparent from (1), a space-group element G when applied to a spin arrangement acts simultaneously both on the components of the spin and on the coordinates of the magnetic atoms. Denoting the operator corresponding to $G = (R|\mathbf{v})$ by $[R\|R|\mathbf{v}]$ explicitly shows this and is to be understood as follows: The rotation on the left-hand side of the double vertical lines acts only in spin space, on the components of the spins. The rotation and translation on the right-hand side act only in 'physical space' (the Euclidean point space in which the atoms are located) on the coordinates of the atoms.

We introduce a new notation for space-group elements similar to the above operator notation. If the operator in (1) corresponding to a space-group element

G is denoted by $[R\|R|\mathbf{v}]$, we denote G by $(R\|R|\mathbf{v})$. Characteristic of space-group elements in this notation is that the same rotation R appears on both the right and left-hand sides of the double vertical lines. This follows directly from (1) and means simply that when applying a space-group element to a spin arrangement, the rotation R acts simultaneously both on the components of the spins and on the coordinates of the atoms.

Spins have the property of changing sign under time inversion. Time inversion when applied to a spin arrangement acts only in spin space, on the components of the spins, and is denoted by $(E'\|E|0)$ where E' is time inversion. Thus, applying time inversion to a spin arrangement means replacing $\mathbf{S}(\mathbf{r})$ by the spin arrangement denoted by $[E'\|E|0]\mathbf{S}(\mathbf{r})$ where $[E'\|E|0]\mathbf{S}(\mathbf{r}) = -\mathbf{S}(\mathbf{r})$. In addition to space-group elements $(R\|R|\mathbf{v})$, one can define elements $(E'R\|R|\mathbf{v})$, *i.e.* products of time-inversion and space-group elements. Elements of the form $(R\|R|\mathbf{v})$ and $(E'R\|R|\mathbf{v})$, excluding the time-inversion element $(E'\|E|0)$, are called magnetic elements.

We now introduce a generalization of the concept of symmetry elements of a spin arrangement by considering in addition to time inversion and the rotations R of the spin space induced by the space-group elements, see (1), still other transformations of the spin space. Let R(3) denote the Euclidean rotation group. An arbitrary element $\mathscr{R}$ of R(3) is a proper or improper rotation matrix which when applied to a spin arrangemnt is defined to act only in spin space, on the components of the spins, and is therefore denoted by $(\mathscr{R}\|E|0)$. Applying an element of R(3) to a spin arrangement means replacing $\mathbf{S}(\mathbf{r})$ by the spin arrangement $[\mathscr{R}\|E|0]\mathbf{S}(\mathbf{r})$ defined by

$$[\mathscr{R}\|E|0]S^i(\mathbf{r}) = \sum_{j=1}^{3} \delta_{\mathscr{R}} \mathscr{R}_{ij} S^i(\mathbf{r}) \tag{2}$$

where $\delta_{\mathscr{R}} = \det \mathscr{R}$ and $i = 1,2,3$.

Within this generalization we define, in addition to elements $(R\|R|\mathbf{v})$ and $(E'R\|R|\mathbf{v})$, elements $(\mathscr{R}R\|R|\mathbf{v})$ and $(E'\mathscr{R}R\|R|\mathbf{v})$. These elements are products of $(\mathscr{R}\|E|0)$ and $(E'\mathscr{R}\|E|0)$ and space-group elements. Since $\mathscr{R}$ is an arbitrary matrix of R(3), and a rotation R induced in spin space by a space-group element is also a matrix of R(3), we can write these elements as $(\mathscr{R}\|R|\mathbf{v})$ and $(E'\mathscr{R}\|R|\mathbf{v})$. From (1) and (2), applying an element $(\mathscr{R}\|R|\mathbf{v})$ to a spin arrangement means replacing $\mathbf{S}(\mathbf{r})$ by the spin arrangement $[\mathscr{R}\|R|\mathbf{v}]\mathbf{S}(\mathbf{r})$ defined by

$$[\mathscr{R}\|R|\mathbf{v}]S^i(\mathbf{r}) = \sum_{j=1}^{3} \delta_{\mathscr{R}} \mathscr{R}_{ij} S^j((R|\mathbf{v})^{-1}\mathbf{r}) \,. \tag{3}$$

Such elements when applied to a spin arrangement act in both the spin space and physical space, *i.e.* on both the components of the spins and the coordinates of the atoms. But, unlike space-group elements, the rotations acting in the two spaces are not necessarily the same. Only if $\mathscr{R} = R$ is $(\mathscr{R}\|R|\mathbf{v})$ a space-group element.

Elements of the form $(\mathscr{R}\|R|\mathbf{v})$ and $(E'\mathscr{R}\|R|\mathbf{v})$ could be called 'spin-space–physical-space elements' but for conciseness will be called simply 'spin elements'. Groups of such elements which leave a spin arrangement invarient could be called 'spin-space–physical-space groups', but again for conciseness will be called 'spin groups'. Spin-space groups, spin translation groups and spin point groups designate spin groups in which the transformations acting in the physical space constitute, respectively, a space group, translation group, and point group. The theory of spin space groups will be considered elsewhere (Litvin & Opechowski, 1973). In this paper we limit our discussion to spin translation groups which will be dealt with below.

For examples of spin elements which are symmetry elements of spin arrangements, we consider the spin arrangements of nickel and of dysprosium. The space group of the atom arrangement in nickel is $\mathsf{G} = Fm3m$ and the spin arrangement is ferromagnetic with spins along the z direction (Kubac, 1972). Applying a spin element $(E\|R|\mathbf{v})$ to the nickel spin arrangement, where the rotation and translation are in G, we have from (3) that

$$[E\|R|\mathbf{v}]\mathbf{S}(\mathbf{r}) = \mathbf{S}((R|\mathbf{v})^{-1}\mathbf{r})$$

which is equal to $\mathbf{S}(\mathbf{r})$ since in a ferromagnetic spin arrangement the magnitude and orientation of the spins of all magnetic atoms are identical. The spin element $(E\|R|\mathbf{v})$ is consequently a symmetry element of this spin arrangement. Such spin elements, *i.e.* the identity rotation acting on the components of the spins in combination with a rotation and translation acting on the coordinates of the atoms, are characteristic symmetry elements of ferromagnetic spin arrangements.

The high-temperature spin arrangement of dysprosium is a helical spin arrangement with all spins perpendicular to the z direction and such that $\mathbf{S}(\mathbf{r}+\mathbf{t}) = \mathscr{R}\mathbf{S}(\mathbf{r})$. $\mathbf{t} = (001)$ and $\mathscr{R}$ denotes a rotation about the z axis through an angle of between 26·5° and 53·2° depending on the temperature (Miwa & Yosida, 1961). Consequently, the dysprosium spin arrangement is invariant under the spin element $(\mathscr{R}\|E|\mathbf{t})$. Such spin elements, a rotation of the spins combined with a translation of the atom positions, are called spin translations and are characteristic symmetry elements of helical spin arrangements.

3. Spin translation groups

Let T denote a crystallographic translation group generated by the three translations $\mathbf{a}_i$ $i = 1,2,3$, and $\mathsf{A} \times \mathsf{R}^+(3)$ the direct product of the time-inversion group A, consisting of identity and time inversion, and the group of proper Euclidean rotations. A spin translation group, denoted by T_s, is defined as a group generated by the three spin translations $(P(\mathbf{a}_i)\|E|\mathbf{a}_i)$ $i = 1,2,3$ where the $P(\mathbf{a}_i)$ are elements of $\mathsf{A} \times \mathsf{R}^+(3)$. A spin translation group T_s will be said to belong to a family of T and P if $\mathbf{a}_i$, $i = 1,2,3$ generate the group T and $P(\mathbf{a}_i)$ $i = 1,2,3$ the group P (Litvin & Opechowski, 1973). An arbitrary element of T_s is denoted by $(P(\mathbf{t})\|E|\mathbf{t})$ where $\mathbf{t} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$ is a translation of

T and $P(\mathbf{t})=P(\mathbf{a}_1)^{n_1}P(\mathbf{a}_2)^{n_2}P(\mathbf{a}_3)^{n_3}$ is an element of the group P. An element of P will be called unprimed if it is an element of $\mathsf{R}^+(3)$, and primed if it is the product of time inversion E' and an element of $\mathsf{R}^+(3)$. A spin translation group will also be denoted by $[P(\mathbf{a}_1), P(\mathbf{a}_2), P(\mathbf{a}_3)]$, a notation in which the generators of T_s explicitly appear.

We will classify all spin translation groups first into crystal systems and then into equivalence classes, called Bravais classes of spin translation groups, in a manner similar to the classification of crystallographic translation groups into seven crystal systems and fourteen Bravais classes. For this purpose we define the holohedry H_s of a spin translation group.

Let P be an element of $\mathsf{A}\times\mathsf{R}(3)$ and H an element of $\mathsf{R}(3)$. The holohedry H_s of a spin translation group is defined as the group of elements $(P\|H|0)$ such that for every element $(P(\mathbf{t})\|E|\mathbf{t})$ of T_s,

$$(P\|H|0)\,(P(\mathbf{t})\|E|\mathbf{t})\,(P\|H|0)^{-1}=(PP(\mathbf{t})P^{-1}\|E|H\mathbf{t}) \quad (4)$$

is also an element of T_s. An element $(P\|H|0)$ belongs to the holohedry of the spin translation group $[P(\mathbf{a}_1), P(\mathbf{a}_2), P(\mathbf{a}_3)]$ if and only if $(PP(\mathbf{a}_i)P^{-1}\|E|H\mathbf{a}_i)$ $i=1,2,3$ are elements of T_s. A holohedry H_s is said to belong to a family of H if the distinct elements H of the elements $(P\|H|0)$ of H_s form the group H. From (4) we note that if $(P\|H|0)$ is an element of H_s then $H\mathbf{t}$ is a translation belonging to T. Therefore H is one of the 32 crystallographic point groups.

We now show that the holohedry of any spin translation group contains at least one element of the form $(P\|I|0)$ where I denotes inversion. Since a spin translation group T_s belonging to a family of T and P is a group, and T is an abelian group, the elements of P commute, and T_s is also an abelian group. Therefore, the elements $P(\mathbf{a}_i)$ $i=1,2,3$ of the generators of a spin translation group fall into one of the following three categories:

1) They are all primed or unprimed rotations about the same axis.
2) They are all twofold primed or unprimed rotations about two or three mutually perpendicular axes.
3) Two are twofold primed or unprimed rotations about perpendicular axes and the third is identity or time inversion.

If T_s is a spin translation group with $P(\mathbf{a}_i)$ coming under the first category, then $(2_\perp\|I|0)$ is an element of its holohedry, where $2_\perp$ denotes a twofold rotation about an axis perpendicular to the rotation axis of the $P(\mathbf{a}_i)$. If T_s is a spin translation group with $P(\mathbf{a}_i)$ coming under the second or third category, then $(E\|I|0)$ is an element of its holohedry. Consequently a holohedry H_s of a spin translation group belongs to a family of H where H is one of the seven crystallographic point groups $\bar{1}$, $2/m$, mmm, $4/mmm$, $\bar{3}m$, $6/mmm$ and $m3m$. We can therefore classify spin translation groups into seven crystal systems according to the point group H of their holohedries. We will use the same nomenclature for spin translation groups, *i.e.* triclinic, monoclinic, orthorhombic *etc.*, as is used in the classification of crystallographic translation groups into seven crystal systems. For example, a spin translation group with holohedry belonging to a family of $\mathsf{H}=4/mmm$ will be called a tetragonal spin translation group.

We now classify spin translation groups into Bravais classes in a manner similar to that of the classification of magnetic translation groups given by Opechowski & Guccione (1965). Let $\mathsf{T}_s(E)$ denote the subgroup of a spin translation group T_s consisting of all elements $(P(\mathbf{t})\|E|\mathbf{t})$ where $P(\mathbf{t})=E$; $\mathsf{H}_s\wedge\mathsf{T}_s$ denote the semi-direct product of a spin translation group and its holohedry. Two spin translation groups T_{s1} with holohedry H_{s1} and T_{s2} with holohedry H_{s2} will be said to belong to the same Bravais class of spin translation groups if (1) the semi-direct product $\mathsf{H}_{s1}\wedge\mathsf{T}_{s1}$ is isomorphic to the semi-direct product $\mathsf{H}_{s2}\wedge\mathsf{T}_{s2}$, (2) the unprimed elements of $\mathsf{H}_{s1}\wedge\mathsf{T}_{s1}$ correspond under the isomorphism to the unprimed elements of $\mathsf{H}_{s2}\wedge\mathsf{T}_{s2}$, and (3) the elements of $\mathsf{T}_{s1}(E)$ correspond under the isomorphism to the elements of $\mathsf{T}_{s2}(E)$.

In this classification two spin translation groups $\mathsf{T}_{s1}=[P(\mathbf{a}_1), P(\mathbf{a}_2), P(\mathbf{a}_3)]$ belonging to a family of T_1, and $\mathsf{T}_{s2}=[P(\mathbf{b}_1), P(\mathbf{b}_2), P(\mathbf{b}_3)]$ belonging to a family of T_2, belong to the same Bravais class of spin translations if $P(\mathbf{a}_i)=P(\mathbf{b}_i)$ $i=1,2,3$ and T_1 and T_2 belong to the same Bravais class of crystallographic translation groups with $\mathbf{a}_i$ corresponding to $\mathbf{b}_i$ $i=1,2,3$. Two spin translation groups $\mathsf{T}_{s1}=[P_1(\mathbf{a}_1), P_1(\mathbf{a}_2), P_1(\mathbf{a}_3)]$ and $\mathsf{T}_{s2}=[P_2(\mathbf{a}_1), P_2(\mathbf{a}_2), P_2(\mathbf{a}_3)]$ both belonging to the same family of T and with the $P_i(\mathbf{a}_i)$ and the $P_2(\mathbf{a}_i)$ both belonging to the same category of rotations, belong to the same Bravais class of spin translation groups if the corresponding elements $P_1(\mathbf{a}_i)$ and $P_2(\mathbf{a}_i)$ are primed or unprimed rotations through the same angle but about different axes. Consequently, in the notation of a representative spin translation of each Bravais class one does not need to denote the absolute orientation of the rotation axes of the elements $P(\mathbf{a}_i)$ $i=1,2,3$, *i.e.* the orientation of the rotation axes with respect to the crystal coordinate system in which the translations of T are defined, but only their mutual orientation.

A representative spin translation group of each Bravais class of spin translation groups is listed in Table 1. The Table is divided into seven headings corresponding to the seven crystal systems of spin translation groups. We give the conditions, if any, on the mutual orientation and magnitude of the generating translations of T due to H, and the representative spin translation groups are listed in the notation $(P_1P_2P_3)$ where $P_i=P(\mathbf{a}_i)$ $i=1,2,3$. A rotation P_i through an angle $2\pi/Z$, where Z is an irrational number, is denoted by Z. N/p denotes a rotation through an angle of $2\pi p/N$, where N is an integer greater than two, p is an integer less than $N/2$ and where N and p are relatively prime. A single symbol Q will be used in Table 1 to denote both an arbitrary Z and an arbitrary N/p. A twofold rotation is denoted by 2 and identity by 1. If two or more different Q appear in the notation of a representative spin translation group, *e.g.* the triclinic $(Q_1Q_2Q_3)$, the corresponding Z's or N's are relatively prime. In the triclinic and monoclinic systems, $(Q_1Q_2 2)$, $(Q\,2\,1)$, $(Q\,2\,2)$, $(Q\,Q^{-1}2)$, and $(2\,2\,Q)$ are such that if $Q=N/p$ then N is an odd integer. A primed symbol denotes that time inversion is combined with the rotation. If not otherwise specified, all three P_i, $i=1,2,3$ denote primed or unprimed rotations about a single arbitrarily oriented axis. If the rotations are not all about a single axis subscripts have been added only to indicate the mutual orientation of the twofoldaxes.

4. Spin translation groups and possible reflexions

The standard formula used to calculate the magnetic contribution to the intensity of unpolarized neutrons elastically scattered from a single crystal, denoted by $\sigma(\mathbf{K})$, is

$$\sigma(\mathbf{K})=|\mathbf{P}(\mathbf{K})|^2-|\hat{\mathbf{K}}\,.\,\mathbf{P}(\mathbf{K})|^2 \qquad (5)$$

where $\mathbf{K}$ is the scattering vector and:

$$\mathbf{P}(\mathbf{K})=\sum_i f_i(\mathbf{K})\mathbf{S}(\mathbf{r}_i)\exp(i\mathbf{K}\,.\,\mathbf{r}_i)\,. \qquad (6)$$

Table 1. *Bravais classes of spin translation groups*

Detailed explanation of the symbols used is given in the final paragraph of § 3.

Triclinic H = $\bar{1}$

Triclinic primitive: No conditions on $\mathbf{a}_1$, $\mathbf{a}_2$, and $\mathbf{a}_3$

$(Q\ 1\ 1)$	$(2\ 1\ 1)$	(2_x2_y1)	$(1\ 1\ 1)$	$(Q_1Q_2 1)$	$(Q_1Q_2 2)$	$(Q\ 2\ 1)$	$(Q_1Q_2Q_3)$
$(Q'1\ 1)$	$(2'1\ 1)$	$(2'_x2_y1)$	$(1\ 1\ 1')$	$(Q'_1Q_2 1)$	$(Q'_1Q_2 2)$	$(Q'2\ 1)$	$(Q'_1Q_2Q_3)$
$(Q\ 1\ 1')$	$(2\ 1\ 1')$	$(2_x2_y1')$		$(Q_1Q_2 1')$	$(Q_1Q_2 2')$	$(Q\ 2'1)$	$(Q'_1Q'_2Q_3)$
				$(Q'_1Q^{1}_{2} 1)$	$(Q'_1Q^{1}_{2} 2)$	$(Q\ 2\ 1')$	$(Q'_1Q'_2Q'_3)$
					$(Q'_1Q_2 2')$	$(Q'2'1)$	
					$(Q'_1Q^{1}_{2} 2')$		

Monoclinic H = $2/m$

Monoclinic primitive: $\mathbf{a}_3$ perpendicular to $\mathbf{a}_1$ and $\mathbf{a}_2$

$(Q\ 1\ 2)$	$(Q\ 1\ 1)$	$(2\ 1\ Q)$	$(2\ 1\ 2)$	$(2\ 1\ 1)$	$(2_x2_y2_x)$	$(2_x1\ 2_y)$
$(Q'1\ 2)$	$(Q'1\ 1)$	$(2'1\ Q)$	$(2'1\ 2)$	$(2'1\ 1)$	$(2'_x2_y2_x)$	$(2'_x1\ 2_y)$
$(Q\ 1'2)$	$(Q\ 1'1)$	$(2\ 1'Q)$	$(2\ 1'2)$	$(2\ 1'1)$	$(2_x2'_y2_x)$	$(2_x1'2_y)$
$(Q\ 1\ 2')$	$(Q\ 1\ 1')$	$(2\ 1\ Q')$	$(2\ 1\ 2')$	$(2\ 1\ 1')$	$(2_x2_y2'_x)$	$(2_x1\ 2'_y)$
$(Q'1\ 2')$	$(Q'1\ 1')$	$(2'1\ Q')$	$(2'1\ 2')$	$(2'1\ 1')$	$(2'_x2_y2'_x)$	$(2'_x1\ 2'_y)$
$(Q\ 1'2')$	$(Q\ 1'1')$	$(2\ 1'Q')$	$(2\ 1'2')$	$(2\ 1'1')$	$(2_x2'_y2'_x)$	$(2_x1'2'_y)$

$(1\ 1\ Q)$	$(1\ 1\ 2)$	(2_x2_y1)	$(1\ 1\ 1)$	$(Q\ 2\ 1)$	$(Q\ 2\ 2)$	$(Q_1Q_2 1)$	$(Q_1Q_2 2)$
$(1'1\ Q)$	$(1'1\ 2)$	$(2'_x2_y1)$	$(1'1\ 1)$	$(Q'2\ 1)$	$(Q'2\ 2)$	$(Q'_1Q_2 2)$	$(Q'_1Q_2 2)$
$(1\ 1Q')$	$(1\ 1\ 2')$	$(2_x2_y1')$	$(1\ 1\ 1')$	$(Q\ 2'1)$	$(Q\ 2'2)$	$(Q_1Q_2 1')$	$(Q_1Q_2 2')$
$(1'1'Q')$	$(1'1'2')$	$(2'_x2_y1')$	$(1'1\ 1')$	$(Q\ 2\ 1')$	$(Q\ 2\ 2')$	$(Q'_1Q'_2 1)$	$(Q'_1Q'_2 2)$
				$(Q'2'1)$	$(Q'2'2)$	$(Q'_1Q_2 1')$	$(Q'_1Q'_2 2')$
				$(Q'2\ 1')$	$(Q'2\ 2')$	$(Q'_1Q'_2 1')$	$(Q'_1Q'_2 2')$
				$(Q\ 2'1')$	$(Q\ 2'2')$		
				$(Q'2'1')$	$(Q'2'2')$		

Monoclinic side-centred: $\mathbf{a}_1+\mathbf{a}_2$ perpendicular to $\mathbf{a}_1-\mathbf{a}_2$ and $\mathbf{a}_3$

$(1\ 1\ Q)$	$(1\ 1\ 2)$	$(Q\ Q\ 1)$	$(Q\ Q^{-1}1)$	$(Q\ Q\ 2)$	$(2\ 2\ 1)$	$(2_x2_x2_y)$
$(1'1'Q)$	$(1'1'2)$	$(Q'Q'1)$	$(Q'Q^{-1\prime}1)$	$(Q'Q'2)$	$(2'2'1)$	$(2'_x2'_x2_y)$
$(1\ 1\ Q')$	$(1\ 1\ 2')$	$(Q\ Q\ 1')$	$(Q\ Q^{-1}1')$	$(Q\ Q\ 2')$	$(2\ 2\ 1')$	$(2_x2_x2^{1}_{y})$
$(1'1'Q')$	$(1'1'2')$					

$(2\ 2\ Q)$	$(Q\ Q^{-1}2)$	$(Q_1Q_1^{-1}Q_2)$	(2_x2_y1)	$(1\ 1\ 1)$
$(2'2'Q)$	$(Q'Q^{-1\prime}2)$	$(Q'_1Q_1^{-1\prime}Q_2)$	$(2'_x2'_y1)$	$(1'1'1)$
$(2\ 2\ Q')$	$(Q\ Q^{-1}2')$	$(Q_1Q_1^{-1}Q'_2)$	$(2_x2_y1')$	$(1\ 1\ 1')$
$(2'2'Q')$	$(Q'Q^{-1\prime}2')$	$(Q'_1Q_1^{-1\prime}Q'_2)$		

Orthorhombic H = mm

Orthorhombic primitive: $\mathbf{a}_1$, $\mathbf{a}_2$, and $\mathbf{a}_3$ are mutually perpendicular

$(1\ 2\ Q)$	$(1\ 1\ Q)$	$(2\ 2\ Q)$	$(2\ 2\ 1)$	$(1\ 1\ 2)$	$(2_x2_x2_z)$	(2_x2_y1)
$(1'2\ Q)$	$(1'1\ Q)$	$(2'2\ Q)$	$(2'2\ 1)$	$(1'1\ 2)$	$(2'_x2_x2_z)$	$(2'_x2_y1)$
$(1\ 2'Q)$	$(1'1'Q)$	$(2'2'Q)$	$(2'2'1)$	$(1'1'2)$	$(2'_x2'_x2_z)$	$(2'_x2'_y1)$
$(1\ 2\ Q')$	$(1\ 1\ Q')$	$(2\ 2\ Q')$	$(2\ 2\ 1')$	$(1\ 1\ 2')$	$(2_x2_x2'_z)$	$(2_x2_y1')$
$(1'2'Q)$	$(1'1\ Q')$	$(2'2\ Q')$	$(2'2\ 1')$	$(1'1\ 2')$	$(2'_x2_x2'_z)$	$(2'_x2_y1')$
$(1'2\ Q')$	$(1'1'Q')$	$(2'2'Q')$	$(2'2'1')$	$(1'1'2')$	$(2'_x2'_x2'_z)$	$(2'_x2'_y1')$
$(1\ 2'Q')$						
$(1'2'Q')$						

		$(2\ 2\ 2)$	$(1\ 1\ 1)$			
		$(2\ 2\ 2')$	$(1\ 1\ 1')$			
		$(2'2'2)$	$(1'1'1)$			
		$(2'2'2')$	$(1'1'1')$			

Table 1 (*cont.*)

Orthorhombic base-centred: $\mathbf{a}_1+\mathbf{a}_2$, $\mathbf{a}_1-\mathbf{a}_2$, and $\mathbf{a}_3$ are mutually perpendicular.

$(Q\ Q\ 1)$	$(Q\ Q\ 2)$	$(1\ 1\ Q)$	$(2\ 2\ Q)$	$(2\ 2\ 1)$	$(1\ 1\ 2)$	$(2\ 2\ 2)$
$(Q'Q'1)$	$(Q'Q'2)$	$(1'1'Q)$	$(2'2'Q)$	$(2'2'1)$	$(1'1'2)$	$(2'2'2)$
$(Q\ Q\ 1')$	$(Q\ Q\ 2')$	$(1\ 1\ Q')$	$(2\ 2\ Q')$	$(2\ 2\ 1')$	$(1\ 1\ 2')$	$(2\ 2\ 2')$
$(Q'Q'1')$	$(Q'Q'2')$	$(1'1'Q')$	$(2'2'Q')$	$(2'2'1')$	$(1'1'2')$	$(2'2'2')$

$(2_x2_x2_y)$	(2_x2_y1)	$(2_x2_y2_z)$	$(1\ 1\ 1)$
$(2'_x2'_x2_y)$	$(2'_x2'_y1)$	$(2'_x2'_y2_z)$	$(1'1'1)$
$(2_x2_x2'_y)$	$(2_x2_y1')$	$(2_x2_y2'_z)$	$(1\ 1\ 1')$
$(2'_x2'_x2'_y)$	$(2'_x2'_y1')$	$(2'_x2'_y2'_z)$	$(1'1'1')$

Orthorhombic body-centred: $\mathbf{a}_1=\frac{1}{2}(-a,b,c)$, $\mathbf{a}_2=\frac{1}{2}(a,-b,c)$, $\mathbf{a}_3=\frac{1}{2}(a,b,-c)$

$(Q\ Q\ Q^{-1})$	$(2\ 2\ 2)$	$(2_x2_x2_y)$	$(1\ 1\ 1)$
$(Q'Q'Q^{-1\prime})$	$(2'2'2')$	$(2'_x2'_x2'_y)$	$(1'1'1')$

Orthorhombic face-centred: $\mathbf{a}_1=\frac{1}{2}(a,b,0)$, $\mathbf{a}_2=\frac{1}{2}(-a,b,0)$, $\mathbf{a}_3=\frac{1}{2}(0,b,c)$

$(2\ 2\ Q)$	$(1\ 1\ Q)$	$(1\ 1\ 2)$	$(2_x2_x2_y)$	$(1\ 1\ 1)$
$(2'2'Q)$	$(1'1'Q)$	$(1'1'2)$	$(2_x2_x2'_y)$	$(1\ 1\ 1')$
$(2\ 2\ Q')$	$(1\ 1\ Q')$	$(1\ 1\ 2')$		

Tetragonal $\mathsf{H}=4/mm$

Tetragonal primitive: $\mathbf{a}_1,\mathbf{a}_2,\mathbf{a}_3$ are mutually perpendicular $a_1=a_2$

$(2\ 2\ Q)$	$(1\ 1\ Q)$	$(2\ 2\ 1)$	$(1\ 1\ 2)$	$(2\ 2\ 2)$	$(2_x2_x2_y)$
$(2'2'Q)$	$(1'1'Q)$	$(2'2'1)$	$(1'1'2)$	$(2'2'2)$	$(2'_x2'_x2_y)$
$(2\ 2\ Q')$	$(1\ 1\ Q')$	$(2\ 2\ 1')$	$(1\ 1\ 2')$	$(2\ 2\ 2')$	$(2_x2_x2'_y)$
$(2'2'Q')$	$(1'1'Q')$	$(2'2'1')$	$(1'1'2')$	$(2'2'2')$	$(2'_x2'_x2'_y)$

(2_x2_y1)	$(2_x2_y2_z)$	$(1\ 1\ 1)$
$(2'_x2'_y1)$	$(2'_x2'_y2_z)$	$(1'1'1)$
$(2_x2_y1')$	$(2_x2_y2'_z)$	$(1\ 1\ 1')$
$(2'_x2'_y1')$	$(2'_x2'_y2'_z)$	$(1'1'1')$

Tetragonal body-centred: $\mathbf{a}_1=\frac{1}{2}(-a,a,c)$, $\mathbf{a}_2=\frac{1}{2}(a,-a,c)$, $\mathbf{a}_3=\frac{1}{2}(a,a,-c)$

$(Q\ Q\ Q^{-1})$	$(2\ 2\ 2)$	$(2_x2_x2_y)$	$(1\ 1\ 1)$
$(Q'Q'Q^{-1\prime})$	$(2'2'2')$	$(2'_x2'_x2'_y)$	$(1'1'1')$

Rhombohedral $\mathsf{H}=\bar{3}m$

Rhombohedral primitive: $a_1=a_2=a_3$ $\mathbf{a}_1 . \mathbf{a}_2=\mathbf{a}_2 . \mathbf{a}_3=\mathbf{a}_1 . \mathbf{a}_3$

$(Q\ Q\ Q)$	$(2\ 2\ 2)$	$(2_x2_y2_z)$	$(1\ 1\ 1)$
$(Q'Q'Q')$	$(2'2'2')$	$(2'_x2'_y2'_z)$	$(1'1'1')$

Hexagonal $\mathsf{H}=6/mm$

Hexagonal primitive: $\mathbf{a}_3$ perpendicular to $\mathbf{a}_1$ and $\mathbf{a}_2$, $a_1=a_2$, and $\mathbf{a}_1 . \mathbf{a}_2=a_1a_2\cos(120°)$

$(1\ 1\ Q)$	$(1\ 1\ 2)$	(2_x2_y1)	$(3\ 3\ 1)$	$(3\ 3\ 2)$	$(3\ 3^{-1}1)$
$(1\ 1\ Q')$	$(1\ 1\ 2')$	$(2_x2_y1')$	$(3\ 3\ 1')$	$(3\ 3\ 2')$	$(3\ 3^{-1}1')$
		$(3\ 3^{-1}2)$	$(1\ 1\ 1)$		
		$(3\ 3^{-1}2')$	$(1\ 1\ 1')$		

Cubic $\mathsf{H}=m3m$

Cubic primitive: $\mathbf{a}_1,\mathbf{a}_2,\mathbf{a}_3$, are mutually perpendicular $a_1=a_2=a_3$

$(2\ 2\ 2)$	$(2_x2_y2_z)$	$(1\ 1\ 1)$
$(2'2'2')$	$(2'_x2'_y2'_z)$	$(1'1'1')$

Cubic body-centred: $\mathbf{a}_1=\frac{1}{2}(-a,a,a)$, $\mathbf{a}_2=\frac{1}{2}(a,-a,a)$, $\mathbf{a}_3=\frac{1}{2}(a,a,-a)$

$(2\ 2\ 2)$	$(1\ 1\ 1)$
$(2'2'2')$	$(1'1'1')$

Cubic face-centred: $\mathbf{a}_1=\frac{1}{2}(a,a,0)$, $\mathbf{a}_2=\frac{1}{2}(0,a,a)$, $\mathbf{a}_3=\frac{1}{2}(a,0,a)$

$(2_x2_y2_z)$	$(1\ 1\ 1)$

$\mathbf{S}(\mathbf{r}_i)$ is the spin and f_i the scattering amplitude of the magnetic atom at position $\mathbf{r}_i$, and the sum is over all magnetic atoms in the crystal. Relation (5) can be made plausible using the quantum mechanical formula given by Halpern & Johnson (1939).

For a spin arrangement invariant under a spin translation group T_s belonging to a family of T, we will find the values of the scattering vector $\mathbf{K}$ for which the intensity $\sigma(\mathbf{K})$ can possibly be non-zero. These values of $\mathbf{K}$ determine the 'possible reflexions' of the neutron scattering. For such a spin arrangement we can rewrite (6) as

$$\mathbf{P}(\mathbf{K})=\sum_{j=1}^{m} f_j(\mathbf{K}) \exp(i\mathbf{K} . \mathbf{r}_j) \sum_{t} \mathbf{S}(\mathbf{r}_j+\mathbf{t}) \exp(i\mathbf{K} . \mathbf{t}) \tag{7}$$

where the sum is over the translations $\mathbf{t}$ of T and the magnetic atoms $j=1 \ldots m$ in the primitive unit cell of

T. The mutual orientation of the spins $\mathbf{S}(\mathbf{r}_j+\mathbf{t})$ for each j and all values of $\mathbf{t}$ is determined by the spin translation group T_s. We have $\mathbf{S}(\mathbf{r}_j+\mathbf{t})=P(\mathbf{t})\mathbf{S}(\mathbf{r}_j)$ from the fact that the spin translation $[P(\mathbf{t})||E|\mathbf{t}]$ of T_s is a symmetry element of the spin arrangement. We then rewrite (7) as

$$\mathbf{P}(\mathbf{K})=\sum_{j=1}^{m} f_j(\mathbf{K}) \exp(i\mathbf{K}\cdot\mathbf{r}_j)\mathbf{S}_j(\mathbf{K}) \tag{8}$$

where

$$\mathbf{S}_j(\mathbf{K})=\sum_{\mathbf{t}} P(\mathbf{t})\mathbf{S}(\mathbf{r}_j) \exp(i\mathbf{K}\cdot\mathbf{t})\,. \tag{9}$$

Lastly, assuming that the spins $\mathbf{S}(\mathbf{r}_j)$ are arbitrarily oriented we preform the summation over $\mathbf{t}$. The values of $\mathbf{K}$ for which the sum (9) is non-zero determine the possible reflexions of a spin arrangement invariant under the spin translation group T_s.

For a spin translation group $\mathrm{T}_s=[P(\mathbf{a}_i),P(\mathbf{a}_2),P(\mathbf{a}_3)]$ belonging to a family of T we determine the values of $\mathbf{K}$ such that $\mathbf{S}_j(\mathbf{K})\neq 0$ in terms of a trio of numbers $\{hkl\}$ where $\mathbf{K}=h\mathbf{b}_1+k\mathbf{b}_2+l\mathbf{b}_3$ and where $\mathbf{b}_i$ $i=1,2,3$ are the generators of the reciprocal translation group of T defined by $\mathbf{a}_i\cdot\mathbf{b}_j=2\pi\delta_{ij}$. We also determine the sum $\mathbf{S}_j(\mathbf{K})$ corresponding to these values of $\mathbf{K}$ as a function of the components of the spin $\mathbf{S}(\mathbf{r}_j)$.

We will take the components of $\mathbf{S}(\mathbf{r}_j)$, and of $\mathbf{S}_j(\mathbf{K})$, in an orthogonal coordinate system defined by the rotation axes of $P(\mathbf{a}_i)$ $i=1,2,3$ and not in the crystal coordinate system in which the translations of the crystallographic translation group T are defined. Thus, the components of $\mathbf{S}_j(\mathbf{K})$ will depend on the mutual orientation of the rotation axes of the $P(\mathbf{a}_i)$ $i=1,2,3$ but not on the absolute orientation of these axes with respect to the crystal coordinate system. The components of $\mathbf{S}(\mathbf{r}_j)$, denoted by $S_{\bar{x}}$, $S_{\bar{y}}$, and $S_{\bar{z}}$, are taken in an orthogonal coordinate system where the $\bar{z}$ axis is along the rotation axis of the $P(\mathbf{a}_i)$ $i=1,2,3$ if all rotations are about a single axis. If the elements $P(\mathbf{a}_i)$ $i=1,2,3$ have subscripts indicating the mutual orientation of perpendicular rotation axes, the components of $\mathbf{S}(\mathbf{r}_j)$ are taken in the orthogonal coordinate system defined by these axes.

Substituting $\mathbf{t}=n_1\mathbf{a}_1+n_2\mathbf{a}_2+n_3\mathbf{a}_3$ and $\mathbf{K}=h\mathbf{b}_1+k\mathbf{b}_2+l\mathbf{b}_3$ into (9), $\mathbf{S}_j(\mathbf{K})$ takes the form

$$\mathbf{S}(hkl)=\sum_{n_1n_2n_3} P_1^{n_1}P_2^{n_2}P_3^{n_3}\mathbf{S}(\mathbf{r}) \times \exp[2\pi i(hn_1+kn_2+ln_3)] \tag{10}$$

where $P_i=P(\mathbf{a}_i)$ $i=1,2,3$ and where we have dropped the index j since $\mathbf{S}(\mathbf{r}_j)$ is arbitrary. For a spin translation group T_s belonging to a family of T we have from (10) that the sum $\mathbf{S}(hkl)$ is dependent only on the value of the rotations P_i $i=1,2,3$ and on the mutual orientation of the rotation axes of these elements. The translations of T do not appear explicitly in (10) and in the above convention for the components of $\mathbf{S}(\mathbf{r})$, the components of $\mathbf{S}(hkl)$ are not dependent on the absolute orientation of the rotation axes of the P_i $i=1,2,3$ with respect to the crystal coordinate system. In addition, let $\mathbf{S}_1(hkl)$

Table 2. *The possible reflexions of magnetic neutron scattering from a single crystal tabulated for the spin translation groups*

The fourth column gives the sum (10) for each set of possible reflexions in the notation

$$A=\begin{pmatrix} S_x \\ S_y \\ S_z \end{pmatrix},\quad B=\begin{pmatrix} 0 \\ 0 \\ S_z \end{pmatrix},\quad C=\begin{pmatrix} S_x \\ S_y \\ 0 \end{pmatrix},\quad D=\begin{pmatrix} S_x \\ 0 \\ 0 \end{pmatrix},$$

$$E=\begin{pmatrix} 0 \\ S_y \\ 0 \end{pmatrix},\quad F=\begin{pmatrix} S_x-iS_y \\ -iS_x+S_y \\ 0 \end{pmatrix} \quad\text{and}\quad G=\begin{pmatrix} S_x+iS_y \\ iS_x+S_y \\ 0 \end{pmatrix}$$

T_s	h	k	l	$\mathbf{S}(hkl)$
(1 1 1)	m	n	q	A
(1 1 1′)	m	n	$q+\frac{1}{2}$	A
(1′1′1)	$m+\frac{1}{2}$	$n+\frac{1}{2}$	q	A
(1′1′1′)	$m+\frac{1}{2}$	$n+\frac{1}{2}$	$q+\frac{1}{2}$	A
(2 1 1)	m	n	q	B
	$m+\frac{1}{2}$	n	q	C
(2′1 1)	m	n	q	C
	$m+\frac{1}{2}$	n	q	B
(2 1 1′)	m	n	$q+\frac{1}{2}$	B
	$m+\frac{1}{2}$	n	$q+\frac{1}{2}$	C
(2′1 1′)	m	n	$q+\frac{1}{2}$	C
	$m+\frac{1}{2}$	n	$q+\frac{1}{2}$	B
(2 1′1′)	m	$n+\frac{1}{2}$	$q+\frac{1}{2}$	B
	$m+\frac{1}{2}$	$n+\frac{1}{2}$	$q+\frac{1}{2}$	C
(2′1′1′)	m	$n+\frac{1}{2}$	$q+\frac{1}{2}$	C
	$m+\frac{1}{2}$	$n+\frac{1}{2}$	$q+\frac{1}{2}$	B
(2 2 1)	$m+\frac{1}{2}$	$n+\frac{1}{2}$	q	C
	m	n	q	B
(2 2 1′)	$m+\frac{1}{2}$	$n+\frac{1}{2}$	$q+\frac{1}{2}$	C
	m	n	$q+\frac{1}{2}$	B
(2′2 1)	m	$n+\frac{1}{2}$	q	B
	$m+\frac{1}{2}$	n	q	C
(2′2 1′)	m	$n+\frac{1}{2}$	$q+\frac{1}{2}$	B
	$m+\frac{1}{2}$	n	$q+\frac{1}{2}$	C
(2′2′1)	m	n	q	C
	$m+\frac{1}{2}$	$n+\frac{1}{2}$	q	B
(2′2′1′)	m	n	$q+\frac{1}{2}$	C
	$m+\frac{1}{2}$	$n+\frac{1}{2}$	$q+\frac{1}{2}$	B
(2 2 2)	$m+\frac{1}{2}$	$n+\frac{1}{2}$	$q+\frac{1}{2}$	C
	m	n	q	B
(2 2 2′)	$m+\frac{1}{2}$	$n+\frac{1}{2}$	q	C
	m	n	$q+\frac{1}{2}$	B
(2′2′2)	m	n	$q+\frac{1}{2}$	C
	$m+\frac{1}{2}$	$n+\frac{1}{2}$	q	B
(2′2′2′)	m	n	q	C
	$m+\frac{1}{2}$	$n+\frac{1}{2}$	$q+\frac{1}{2}$	B
(2_x2_y1)	m	$n+\frac{1}{2}$	q	D
	$m+\frac{1}{2}$	n	q	E
	$m+\frac{1}{2}$	$n+\frac{1}{2}$	q	B
$(2'_x2_y1)$	$m+\frac{1}{2}$	$n+\frac{1}{2}$	q	D
	m	n	q	E
	m	$n+\frac{1}{2}$	q	B
$(2_x2_y1')$	m	$n+\frac{1}{2}$	$q+\frac{1}{2}$	D
	$m+\frac{1}{2}$	n	$q+\frac{1}{2}$	E
	$m+\frac{1}{2}$	$n+\frac{1}{2}$	$q+\frac{1}{2}$	B
$(2'_x2_y1')$	$m+\frac{1}{2}$	$n+\frac{1}{2}$	$q+\frac{1}{2}$	D
	m	n	$q+\frac{1}{2}$	E
	m	$n+\frac{1}{2}$	$q+\frac{1}{2}$	B
$(2'_x2'_y1)$	$m+\frac{1}{2}$	n	q	D
	m	$n+\frac{1}{2}$	q	E
	m	n	q	B
$(2'_x2'_y1')$	$m+\frac{1}{2}$	n	$q+\frac{1}{2}$	D
	m	$n+\frac{1}{2}$	$q+\frac{1}{2}$	E
	m	n	$q+\frac{1}{2}$	B
$(2_x2_x2_y)$	m	n	$q+\frac{1}{2}$	D
	$m+\frac{1}{2}$	$n+\frac{1}{2}$	q	E
	$m+\frac{1}{2}$	$n+\frac{1}{2}$	$q+\frac{1}{2}$	B

Table 2 (*cont.*)

T_s	h	k	l	$\mathbf{S}(hkl)$
$(2'_x2_x2_y)$	$m+\frac{1}{2}$	n	$q+\frac{1}{2}$	D
	m	$n+\frac{1}{2}$	q	E
	m	$n+\frac{1}{2}$	$q+\frac{1}{2}$	B
$(2'_x2'_x2_y)$	$m+\frac{1}{2}$	$n+\frac{1}{2}$	$q+\frac{1}{2}$	D
	m	n	q	E
	m	n	$q+\frac{1}{2}$	B
$(2_x2_x2'_y)$	m	n	q	D
	$m+\frac{1}{2}$	$n+\frac{1}{2}$	$q+\frac{1}{2}$	E
	$m+\frac{1}{2}$	$n+\frac{1}{2}$	q	B
$(2_x2'_x2'_y)$	m	$n+\frac{1}{2}$	q	D
	$m+\frac{1}{2}$	n	$q+\frac{1}{2}$	E
	$m+\frac{1}{2}$	n	q	B
$(2'_x2'_x2'_y)$	$m+\frac{1}{2}$	$n+\frac{1}{2}$	q	D
	m	n	$q+\frac{1}{2}$	E
	m	n	q	B
$(2_x2_y2_z)$	m	$n+\frac{1}{2}$	$q+\frac{1}{2}$	D
	$m+\frac{1}{2}$	n	$q+\frac{1}{2}$	E
	$m+\frac{1}{2}$	$n+\frac{1}{2}$	q	B
$(2_x2_y2'_z)$	m	$n+\frac{1}{2}$	q	D
	$m+\frac{1}{2}$	n	q	E
	$m+\frac{1}{2}$	$n+\frac{1}{2}$	$q+\frac{1}{2}$	B
$(2'_x2'_y2_z)$	$m+\frac{1}{2}$	n	$q+\frac{1}{2}$	D
	m	$n+\frac{1}{2}$	$q+\frac{1}{2}$	E
	m	n	q	B
$(2'_x2'_y2'_z)$	$m+\frac{1}{2}$	n	q	D
	m	$n+\frac{1}{2}$	q	E
	m	n	$q+\frac{1}{2}$	B
$(Q\ 1\ 1)$	$m-1/Q$	n	q	F
	$m+1/Q$	n	q	G
	m	n	q	B
$(Q'1\ 1)$	$m+\frac{1}{2}-1/Q$	n	q	F
	$m+\frac{1}{2}+1/Q$	n	q	G
	$m+\frac{1}{2}$	n	q	B
$(Q\ 1\ 1')$	$m-1/Q$	n	$q+\frac{1}{2}$	F
	$m+1/Q$	n	$q+\frac{1}{2}$	G
	m	n	$q+\frac{1}{2}$	B
$(Q'1\ 1')$	$m+\frac{1}{2}-1/Q$	n	$q+\frac{1}{2}$	F
	$m+\frac{1}{2}+1/Q$	n	$q+\frac{1}{2}$	G
	m	n	$q+\frac{1}{2}$	B
$(Q\ 1'1')$	$m-1/Q$	$n+\frac{1}{2}$	$q+\frac{1}{2}$	F
	$m+1/Q$	$n+\frac{1}{2}$	$q+\frac{1}{2}$	G
	m	$n+\frac{1}{2}$	$q+\frac{1}{2}$	B
$(Q'1'1')$	$m+\frac{1}{2}-1/Q$	$n+\frac{1}{2}$	$q+\frac{1}{2}$	F
	$m+\frac{1}{2}+1/Q$	$n+\frac{1}{2}$	$q+\frac{1}{2}$	G
	$m+\frac{1}{2}$	$n+\frac{1}{2}$	$q+\frac{1}{2}$	B
$(Q\ 2\ 1)$	$m-1/Q$	$n+\frac{1}{2}$	q	F
	$m+1/Q$	$n+\frac{1}{2}$	q	G
	m	n	q	B
$(Q\ 2\ 1')$	$m-1/Q$	$n+\frac{1}{2}$	$q+\frac{1}{2}$	F
	$m+1/Q$	$n+\frac{1}{2}$	$q+\frac{1}{2}$	G
	m	n	$q+\frac{1}{2}$	B
$(Q\ 2'1)$	$m-1/Q$	n	q	F
	$m+1/Q$	n	q	G
	m	$n+\frac{1}{2}$	q	B
$(Q\ 2'1')$	$m-1/Q$	n	$q+\frac{1}{2}$	F
	$m+1/Q$	n	$q+\frac{1}{2}$	G
	m	$n+\frac{1}{2}$	$q+\frac{1}{2}$	B
$(Q'2\ 1)$	$m+\frac{1}{2}-1/Q$	$n+\frac{1}{2}$	q	F
	$m+\frac{1}{2}+1/Q$	$n+\frac{1}{2}$	q	G
	$m+\frac{1}{2}$	n	q	B
$(Q'2\ 1')$	$m+\frac{1}{2}-1/Q$	$n+\frac{1}{2}$	$q+\frac{1}{2}$	F
	$m+\frac{1}{2}+1/Q$	$n+\frac{1}{2}$	$q+\frac{1}{2}$	G
	$m+\frac{1}{2}$	n	$q+\frac{1}{2}$	B
$(Q'2'1)$	$m+\frac{1}{2}-1/Q$	n	q	F
	$m+\frac{1}{2}+1/Q$	n	q	G
	$m+\frac{1}{2}$	$n+\frac{1}{2}$	q	B
$(Q'2'1')$	$m+\frac{1}{2}-1/Q$	n	$q+\frac{1}{2}$	F
	$m+\frac{1}{2}+1/Q$	n	$q+\frac{1}{2}$	G
	$m+\frac{1}{2}$	$n+\frac{1}{2}$	q	B

Table 2 (*cont.*)

T_s	h	k	l	$\mathbf{S}(hkl)$
$(Q\ 2\ 2)$	$m-1/Q$	$n+\frac{1}{2}$	$q+\frac{1}{2}$	F
	$m+1/Q$	$n+\frac{1}{2}$	$q+\frac{1}{2}$	G
	m	n	q	B
$(Q\ 2\ 2')$	$m-1/Q$	$n+\frac{1}{2}$	q	F
	$m+1/Q$	$n+\frac{1}{2}$	q	G
	m	n	$q+\frac{1}{2}$	B
$(Q\ 2'2')$	$m-1/Q$	n	q	F
	$m+1/Q$	n	q	G
	m	$n+\frac{1}{2}$	$q+\frac{1}{2}$	B
$(Q'2\ 2)$	$m+\frac{1}{2}-1/Q$	$n+\frac{1}{2}$	$q+\frac{1}{2}$	F
	$m+\frac{1}{2}+1/Q$	$n+\frac{1}{2}$	$q+\frac{1}{2}$	G
	$m+\frac{1}{2}$	n	q	B
$(Q'2\ 2')$	$m+\frac{1}{2}-1/Q$	$n+\frac{1}{2}$	q	F
	$m+\frac{1}{2}+1/Q$	$n+\frac{1}{2}$	q	G
	$m+\frac{1}{2}$	n	$q+\frac{1}{2}$	B
$(Q'2'2')$	$m+\frac{1}{2}-1/Q$	n	q	F
	$m+\frac{1}{2}+1/Q$	n	q	G
	$m+\frac{1}{2}$	$n+\frac{1}{2}$	$q+\frac{1}{2}$	B
(Q_1Q_21)	$m-1/Q$	$n-1/Q$	q	F
	$m+1/Q$	$n+1/Q$	q	G
	m	n	q	B
(Q_1Q_21')	$m-1/Q$	$n-1/Q$	$q+\frac{1}{2}$	F
	$m+1/Q$	$n+1/Q$	$q+\frac{1}{2}$	G
	m	n	$q+\frac{1}{2}$	B
$(Q'_1Q_2\ 1)$	$m+\frac{1}{2}-1/Q_1$	$n-1/Q_2$	q	F
	$m+\frac{1}{2}+1/Q_1$	$n+1/Q_2$	q	G
	m	n	q	B
$(Q'_1Q'_21)$	$m+\frac{1}{2}-1/Q$	$n+\frac{1}{2}-1/Q$	q	F
	$m+\frac{1}{2}+1/Q$	$n+\frac{1}{2}+1/Q$	q	G
	$m+\frac{1}{2}$	$n+\frac{1}{2}$	q	B
$(Q'Q'1')$	$m+\frac{1}{2}-1/Q$	$n+\frac{1}{2}-1/Q$	$q+\frac{1}{2}$	F
	$m+\frac{1}{2}+1/Q$	$n+\frac{1}{2}+1/Q$	$q+\frac{1}{2}$	G
	$m+\frac{1}{2}$	$n+\frac{1}{2}$	$q+\frac{1}{2}$	B
(Q_1Q_22)	$m-1/Q$	$n-1/Q$	$q+\frac{1}{2}$	F
	$m+1/Q$	$n+1/Q$	$q+\frac{1}{2}$	G
	m	n	q	B
(Q_1Q_22')	$m-1/Q$	$n-1/Q$	q	F
	$m+1/Q$	$n+1/Q$	q	G
	m	n	$q+\frac{1}{2}$	B
$(Q'_1Q_2\ 2)$	$m+\frac{1}{2}-1/Q_1$	$n-1/Q_2$	$q+\frac{1}{2}$	F
	$m+\frac{1}{2}+1/Q_1$	$n+1/Q_2$	$q+\frac{1}{2}$	G
	$m+\frac{1}{2}$	n	q	B
$(Q'_1Q_2\ 2')$	$m+\frac{1}{2}-1/Q_1$	$n-1/Q_2$	q	F
	$m+\frac{1}{2}+1/Q_1$	$n+1/Q_2$	q	G
	$m+\frac{1}{2}$	n	$q+\frac{1}{2}$	B
$(Q'_1Q'_22)$	$m+\frac{1}{2}-1/Q$	$n+\frac{1}{2}-1/Q$	$q+\frac{1}{2}$	F
	$m+\frac{1}{2}+1/Q$	$n+\frac{1}{2}+1/Q$	$q+\frac{1}{2}$	G
	$m+\frac{1}{2}$	$n+\frac{1}{2}$	q	B
$(Q'_1Q'_22')$	$m+\frac{1}{2}-1/Q$	$n+\frac{1}{2}-1/Q$	q	F
	$m+\frac{1}{2}+1/Q$	$n+\frac{1}{2}+1/Q$	q	G
	$m+\frac{1}{2}$	$n+\frac{1}{2}$	$q+\frac{1}{2}$	B
$(Q\ Q^{-1}1)$	$m-1/Q$	$n+1/Q$	q	F
	$m+1/Q$	$n-1/Q$	q	G
	m	n	q	B
$(Q\ Q^{-1}1')$	$m-1/Q$	$n+1/Q$	$q+\frac{1}{2}$	F
	$m+1/Q$	$n-1/Q$	$q+\frac{1}{2}$	G
	m	n	$q+\frac{1}{2}$	B
$(Q'Q^{-1'}1)$	$m+\frac{1}{2}-1/Q$	$n+\frac{1}{2}+1/Q$	q	F
	$m+\frac{1}{2}+1/Q$	$n+\frac{1}{2}-1/Q$	q	G
	$m+\frac{1}{2}$	$n+\frac{1}{2}$	q	B
$(Q\ Q^{-1}2)$	$m-1/Q$	$n+1/Q$	$q+\frac{1}{2}$	F
	$m+1/Q$	$n-1/Q$	$q+\frac{1}{2}$	G
	m	n	q	B
$(Q'Q^{-1'}2)$	$m+\frac{1}{2}-1/Q$	$n+\frac{1}{2}-1/Q$	$q+\frac{1}{2}$	F
	$m+\frac{1}{2}+1/Q$	$n+\frac{1}{2}-1/Q$	$q+\frac{1}{2}$	G
	$m+\frac{1}{2}$	$n+\frac{1}{2}$	q	B
$(Q\ Q^{-1}2')$	$m-1/Q$	$n+1/Q$	q	F
	$m+1/Q$	$n-1/Q$	q	G
	m	n	$q+\frac{1}{2}$	B

Table 2 (*cont.*)

T_s	h	k	l	$\mathbf{S}(hkl)$
$(Q'Q^{-1\prime}2')$	$m+\frac{1}{2}-1/Q$	$n+\frac{1}{2}+1/Q$	q	F
	$m+\frac{1}{2}+1/Q$	$n+\frac{1}{2}-1/Q$	q	G
	$m+\frac{1}{2}$	$n+\frac{1}{2}$	$q+\frac{1}{2}$	B
$(Q_1Q_2Q_3)$	$m-1/Q$	$n-1/Q$	$q-1/Q$	F
	$m+1/Q$	$n+1/Q$	$q+1/Q$	G
	m	n	q	B
$(Q'_1Q_2Q_3)$	$m+\frac{1}{2}-1/Q_1$	$n-1/Q_2$	$q-1/Q_3$	F
	$m+\frac{1}{2}+1/Q_1$	$n+1/Q_2$	$q+1/Q_3$	G
	$m+\frac{1}{2}$	n	q	B
$(Q'_1Q'_2Q_3)$	$m+\frac{1}{2}-1/Q_1$	$n+\frac{1}{2}-1/Q_2$	$q-1/Q_3$	F
	$m+\frac{1}{2}+1/Q_1$	$n+\frac{1}{2}+1/Q_2$	$q+1/Q_3$	G
	$m+\frac{1}{2}$	$n+\frac{1}{2}$	q	B
$(Q'_1Q'_2Q'_3)$	$m+\frac{1}{2}-1/Q$	$n+\frac{1}{2}-1/Q$	$q+\frac{1}{2}-1/Q$	F
	$m+\frac{1}{2}+1/Q$	$n+\frac{1}{2}+1/Q$	$q+\frac{1}{2}+1/Q$	G
	$m+\frac{1}{2}$	$n+\frac{1}{2}$	$q+\frac{1}{2}$	B
$(Q_1Q_1^{-1}Q_2)$	$m-1/Q_1$	$n+1/Q_1$	$q-1/Q_2$	F
	$m+1/Q_1$	$n-1/Q_1$	$q+1/Q_2$	G
	m	n	q	B
$(Q'_1Q_1^{-1\prime}Q_2)$	$m+\frac{1}{2}-1/Q_1$	$n+\frac{1}{2}+1/Q_1$	$q-1/Q_2$	F
	$m+\frac{1}{2}+1/Q_1$	$n+\frac{1}{2}-1/Q_1$	$q+1/Q_2$	G
	$m+\frac{1}{2}$	$n+\frac{1}{2}$	q	B
$(Q_1Q_1^{-1}Q'_2)$	$m-1/Q_1$	$n+1/Q_1$	$q+\frac{1}{2}-1/Q_2$	F
	$m+1/Q_1$	$n-1/Q_1$	$q+\frac{1}{2}+1/Q_2$	G
	m	n	$q+\frac{1}{2}$	B
$(Q'_1Q_1^{-1\prime}Q'_2)$	$m+\frac{1}{2}-1/Q_1$	$n+\frac{1}{2}+1/Q_1$	$q+\frac{1}{2}-1/Q_2$	F
	$m+\frac{1}{2}+1/Q_1$	$n+\frac{1}{2}-1/Q_1$	$q+\frac{1}{2}+1/Q_2$	G
	$m+\frac{1}{2}$	$n+\frac{1}{2}$	$q+\frac{1}{2}$	B

denote the sum (10) corresponding to a spin translation group $\mathsf{T}_{s1}=(P_1P_2P_3)$ and $\mathbf{S}_2(hkl)$ the sum corresponding to $\mathsf{T}_{s2}=(\bar{P}_1\bar{P}_2\bar{P}_3)$. Since the elements P_i in (10) commute, if the P_i of T_{s1} are a permutation of the $\bar{P}_i$ of T_{s2}, then

$$\mathbf{S}_1(hkl)=\mathbf{S}_2(\bar{h}\bar{k}\bar{l})$$

where $\bar{h}$, $\bar{k}$, and $\bar{l}$ are a permutation of h, k, and l given by:

$$\begin{pmatrix} hkl \\ \bar{h}\bar{k}\bar{l} \end{pmatrix} = \begin{pmatrix} P_1P_2P_3 \\ \bar{P}_1\bar{P}_2\bar{P}_3 \end{pmatrix} .$$

Consequently, we have listed in Table 2 only distinct triplets of elements P_i $i=1,2,3$ appearing in the notation of the spin translation groups of Table 1, disregarding the order in which these elements appear and the translation group T. For each triplet $(P_1P_2P_3)$ the sets of values of $\{hkl\}$ corresponding to possible reflexions are given; m, n, and q denote arbitrary integers. In addition, $\mathbf{S}(hkl)$ for each set of $\{hkl\}$ is given in terms of the components of the spin $\mathbf{S}(\mathbf{r})$ given in the orthogonal coordinate system defined by the rotation axes of the P_i, $i=1,2,3$ as explained above.

As an example consider the hexagonal spin translation group $(11Q)$. In Table 2 we find the values $\{hkl\}$ corresponding to the trio of elements $(Q11)$. The values of $\mathbf{K}$ corresponding to the possible reflexions of a spin arrangement invariant under the hexagonal spin translation group $(11Q)$ are therefore given by $\{lkh\}$, *i.e.* where the indices h and l have been interchanged. There are three sets of values of $\mathbf{K}$, the first $\{q,n,m\}$ due to the component of the spins $\mathbf{S}(\mathbf{r}+\mathbf{t})$ along the rotation axis of Q, and the remaining two $\{q,n,m\pm 1/Q\}$ due to the rotated components of the spins perpendicular to the rotation axis. The reflexions corresponding to the first set of values of $\mathbf{K}$ are referred to as 'fundamental reflexions' and corresponding to the latter sets as 'satellite reflexions' by Lyons, Kaplan, Dwight & Menyuk (1962).

5. Application to neutron-diffraction analysis

We will show below how by considering the indices of observed magnetic reflexions and the list of possible reflexions given in Table 2 one can determine the spin translation groups which are compatible with the neutron-diffraction data. Such information is of special importance in determining non-collinear spin arrangements because the invariance of a spin arrangement under a spin translation group implies the mutual orientation of non-collinear spins which are related by rotations that are not in the space group of the crystal. (The invariance of a non-collinear spin arrangement under a magnetic space group implies the mutual orientation of only those spins which are related by rotations of the space group of the crystal.) We then show how such information can be utilized in determining the spin arrangement of a magnetic crystal and consider as an example the analysis of neutron diffraction data of chromium selenide.

Consider a crystal with magnetic atoms which form an atom arrangement invariant under the space group G. Let T denote the subgroup of primitive translations of G, a crystallographic translation group belonging to a crystal system characterized by the point group R. The spin translation symmetry group of a spin arrangement defined on the magnetic atoms is a group T_s belonging to a family of T_1 where T_1 is equal to or a subgroup of T, and whose holohedry H_s belongs to a family of H where H is equal to or a subgroup of R.

We consider all such spin translation groups starting with those groups belonging to a family of T with holohedry belonging to a family of R. We choose one such spin translation group T_s belonging to a family of T with holohedry belonging to a family of R and determine if the possible reflexions corresponding to this spin translation group are compatible with the experimentally observed reflexions. To do this we index the observed reflexions with respect to the reciprocal translation group of T, and compare the indices of these reflexions with the indices of the possible reflexions corresponding to T_s given in Table 2. If there are observed reflexions which do not correspond to any of the possible reflexions then we conclude that T_s cannot be the spin translation symmetry group of the spin arrangement which is to be determined. Provided that every observed reflexion corresponds to a possible reflexion, the spin translation group T_s will be said to be compatible with the observed reflexions.

By assuming that T_s is the spin translation symmetry group of the spin arrangement, the mutual orientation of the spins $\mathbf{S}(\mathbf{r}_j+\mathbf{t})$ for fixed j is determined. To uniquely determine the spin arrangement one must in addition find the magnitude of the spins $\mathbf{S}(\mathbf{r}_j), j=1\ldots m$ and their orientation with respect to the crystal's coordinate system. To do this one can consider the mutual orientation of the spins $\mathbf{S}(\mathbf{r}_j+\mathbf{t})$ as additional information to be used in conjunction with the procedure based on the use of magnetic groups, or, if the number m of magnetic atoms in the primitive unit cell defined by T is small, in the following manner. We calculate the intensity $\sigma(\mathbf{K})$ as a function of the m spins $\mathbf{S}(\mathbf{r}_j), j=1\ldots m$ in (8). We then vary the magnitude and orientation of these spins to find values such that the calculated and observed intensities are in agreement. If there exist such values of $\mathbf{S}(\mathbf{r}_j)$, $j=1,\ldots,m$ we have determined the spin arrangement. If not, then we conclude that this spin translation group is not the spin translation symmetry group of the spin arrangement. Only after all possibilities of spin translation groups belonging to the family of T with holohedry belonging to a family of R have been ruled out does one then proceed in the same manner to consider other possible spin translation groups.

As an example of this we consider the analysis of the neutron diffraction data of chromium selenide given by Corliss, Elliott, Hastings & Sass (1961). The chromium-atom arrangement is a simple hexagonal arrangement with one atom per unit cell and space-group symmetry *P*6/*mmm*. The subgroup T of *P*6/*mmm* is a hexagonal crystallographic translation group, *i.e.* R = 6*mmm*.

We first consider spin translation groups T_s belonging to a family of T with holohedry belonging to a family of 6/*mmm*. These are the hexagonal spin translation groups listed in Table 1. The observed magnetic reflexions, indexed with respect to the reciprocal translation group of T are

$$(\tfrac{1}{3}\tfrac{1}{3}\tfrac{1}{2})\quad(\tfrac{2}{3}\tfrac{2}{3}\tfrac{3}{2})$$
$$(\tfrac{2}{3}\tfrac{2}{3}\tfrac{1}{2})\quad(10\tfrac{1}{2})$$

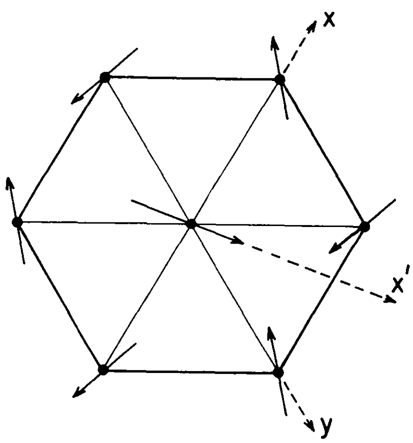

Fig. 1. The 'umbrella' structure of CrSe: the mutual orientations of the spins in the $z=0$ plane are shown. Only the components of the spins in the plane have been drawn.

and the magnetic reflexions (00*l*) are absent (Corliss *et al.*, 1961). From Table 2 we find that the observed reflexions are compatible only with a hexagonal spin translation group belonging to the Bravais class (331′). The possible reflexions corresponding to (331′) are found in Table 2 under (Q_1Q_21') by taking $Q_1=Q_2=3$. Since there is only one chromium atom in the primitive unit cell of T the mutual orientation of all the spins is determined by assuming that (331′) is the spin translation symmetry group of the chromium spin arrangement.

We now calculate the intensities $\sigma(\mathbf{K})$ as a function of the chromium spin $\mathbf{S}(\mathbf{r})$ at $\mathbf{r}=(000)$. Relation (8) becomes

$$\mathbf{P}(\mathbf{K})=\delta\left(\mathbf{K}-\boldsymbol{\tau}-\frac{\mathbf{b}_3}{2}\right)f(\mathbf{K})\begin{pmatrix}0\\0\\S_{\bar{z}}\end{pmatrix}$$
$$+\delta\left(\mathbf{K}-\boldsymbol{\tau}-\frac{\mathbf{b}_1+\mathbf{b}_2}{3}-\frac{\mathbf{b}_3}{2}\right)\tfrac{1}{2}f(\mathbf{K})\begin{pmatrix}S_{\bar{x}}\\-iS_{\bar{x}}\\0\end{pmatrix}$$
$$+\delta\left(\mathbf{K}-\boldsymbol{\tau}-\frac{2(\mathbf{b}_1+\mathbf{b}_2)}{3}-\frac{\mathbf{b}_3}{2}\right)\tfrac{1}{2}f(\mathbf{K})\begin{pmatrix}S_{\bar{x}}\\iS_{\bar{x}}\\0\end{pmatrix}\qquad(11)$$

where $\mathbf{b}_i$, $i=1,2,3$ are the generators of the reciprocal translation group of T and $\boldsymbol{\tau}$ is an arbitrary reciprocal translation. $S_{\bar{z}}$ and $S_{\bar{x}}$ are the components of the spin $\mathbf{S}(\mathbf{r})$ given in an orthogonal coordinate system where the $\bar{z}$ axis is along the rotation axis of the threefold rotations of (331′) and the $\bar{x}$ axis is chosen along the component of the spin perpendicular to the $\bar{z}$ axis. The orientation of this orthogonal coordinate system with respect to the crystals hexagonal coordinate system is as yet undetermined.

The calculated intensities $\sigma(00l)$ are dependent only on the first term of (11) and using (5) are found to be proportional to $S_{\bar{z}}$ $(1-\cos^2\theta)$ where θ is the angle between the $\bar{z}$ axis and the crystal's z axis. Since the observed intensities $\sigma(00l)$ are zero, either $S_{\bar{z}}=0$ or $\cos\theta=1$. Taking $S_{\bar{z}}=0$ would mean that the calculated intensity $\sigma(10\tfrac{1}{2})$ is also zero which is incompatible with the experimentally observed $\sigma(10\tfrac{1}{2})$ reflexion. Therefore $\cos\theta=1$ and the $\bar{z}$ axis coincides with the crystal z axis and the $\bar{x}$ axis is in the basal plane of the hexagonal unit cell.

The calculated intensities are found by substituting (11) into (5). For comparison with neutron-diffraction data obtained from a powder sample we average over all equivalent wave vectors $\mathbf{K}$ and obtain

$$\langle\sigma(\mathbf{K})\rangle=\delta\left(\mathbf{K}-\boldsymbol{\tau}-\frac{\mathbf{b}_3}{2}\right)f(\mathbf{K})^2S_z^2[1-K_z^2]$$
$$+\delta\left(\mathbf{K}-\boldsymbol{\tau}-\frac{\mathbf{b}_1+\mathbf{b}_2}{3}-\frac{\mathbf{b}_3}{2}\right)\tfrac{1}{4}f(\mathbf{K})^2S_{\bar{x}}^2[1+K_z^2]$$
$$+\delta\left(\mathbf{K}-\boldsymbol{\tau}-\frac{2(\mathbf{b}_1+\mathbf{b}_2)}{3}-\frac{\mathbf{b}_3}{2}\right)\tfrac{1}{4}f(\mathbf{K})^2S_{\bar{x}}^2[1+K_z^2]\qquad(12)$$

where K_z is the z component of the unit scattering vector $\hat{\mathbf{K}}$. Varying the values of S_z and $S_{\bar{x}}$ one finds (Corliss *et al.*, 1961) non-zero values such that the calculated intensities are in agreement with the observed. We conclude that the chromium spin arrangement is invariant under the spin translation group (331′) where the rotations are about the z axis. The spins have both a component in the z direction and in the basal plane. This is the so-called 'umbrella' spin arrangement shown in Fig. 1. We note that the spin arrangement has not been uniquely determined since the orientation of the $\bar{x}$ axis with respect to the crystal's hexagonal coordinate system, and consequently of the components of the spins in the basal plane, is unobtainable from the neutron diffraction data.

Relation (12) was also derived by Corliss *et al.* (1961), but only after *ad hoc* assumptions were made pertaining to the rotational symmetry of the spin arrangement. The advantage of applying the theory of spin translation groups in the analysis of neutron diffraction data is that information on the mutual orientation of spin can be obtained, without making any assumptions on the rotational symmetry of the spin arrangement, by using Tables 1 and 2. In fact, relation (12) was derived above by considering only the indices of the magnetic reflexions and the table of possible reflexions of spin translation groups.

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Calculation of the T, L and S Tensors from Crystal Forces and *vice versa*

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It would be useful if the measured values of **T**, **L** and **S** could be used directly to give information about the intermolecular crystalline forces. This requires the assumption of an Einstein model for the molecular dynamics, where **T**, **L** and **S** are related through a smearing function to a molecular site potential function. It is shown that this potential function has no physical interpretation. Einstein-model calculations are compared with the physically justifiable Born–von Kàrmàn calculations for four examples, sulphur, benzene, phenanthrene and pyrene, and very little regularity is apparent in the comparison of these results.

1. Introduction

The average thermal motion of a rigid molecule in a crystal is correctly described by three tensors **T**, **L** and **S** which can be obtained from diffraction experiments. **T** and **L** describe respectively the mean-square translational and librational displacements, while S, first introduced by Schomaker & Trueblood (1968), takes account of the correlations between translation and libration. These tensors derive from averages over all the lattice modes of vibration whose number may be of the order of Avogadro's number. It is therefore unsafe