COMPUTER PROGRAMS

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A computer program to derive (3+1)-dimensional symmetry operations from two-line symbols

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Abstract

A computer program has been written for the derivation of $(3 + 1)$-dimensional symmetry operations from the two-line symbols. The derivation is based on the concept of generators $\{[\Gamma(R_E^\nu),\ \varepsilon^\nu,\ \mathbf{s}^\nu,\ \tau^\nu,\ \mathbf{q}]|\nu = 1,\ \mathrm{NG}\}$, in which $\{[\Gamma(R_E^\nu),\ \mathbf{s}^\nu)|\nu = 1, \mathrm{NG}\}$ denotes the set of generators of the basic space group represented by the upper line. The program, called *SPGR4D*, is written in Fortran77 and based on the program by Burzlaff & Hountas (1982) [*J. Appl. Cryst.* (1982), **15**, 464–467] for the derivation of symmetry operations in three-dimensional space. *SPGR4D* has been incorporated into a new version of the direct-methods program *DIMS* for solving incommensurate modulated crystal structures.

1. Introduction

The multidimensional representation of an incommensurate structure is characterized by the existence of at least four independent translation vectors, three of which describe a conventional three-dimensional lattice, while the additional ones describe the periodicity of modulation and are incommensurate with the first three. Because of the incommensurate property, there is no three-dimensional space-group symmetry. It has been shown, however, that a modulated structure can be depicted as a section through a $(3 + d)$-dimensional periodic structure having a superspace group in $(3 + d)$-dimensional space (de Wolff, 1974, 1977; Janner & Janssen, 1977). For the simplest case, in which there is only one additional dimension, the inequivalent $(3 + 1)$-dimensional superspace groups were found and tabulated for 24 classes of Bravais lattices (de Wolff, Janssen & Janner, 1981). The list was further checked and a few corrections were made by Yamamoto, Janssen, Janner & de Wolff (1985), giving in total 775 inequivalent $(3 + 1)$-dimensional superspace groups. The full classification has also been given for incommensurate crystals with additional dimensions d of less than four. The introduction of multi-dimensional description together with superspace symmetry transformations is important in the structure determination of incommensurate crystals (Yamamoto, 1982). At present, the superspace-group formalism has been widely accepted and used in both classification and structure determination (Janssen, Janner, Looijenga-Vos & de Wolff (1992). A number of multidimensional least-squares programs, *REMOS*, *JANA* and *MSR* [see, respectively, Yamamoto (1991), Petrícek, Malý & Císarová (1991) and Paciorek (1991) and references therein], have been written to solve and/or refine incommensurate modulated structures. A direct-methods program *DIMS* (Fu & Fan, 1994) has been constructed to solve the phase problem of one-dimensional incommensurate structures, which is based on a multidimensional modified Sayre equation (Hao, Liu & Fan, 1987). Up to now, however, most structure-analysis program systems for incommensurate crystals have required the input of multidimensional symmetry operations. This is very inconvenient and can easily cause errors. To avoid this disadvantage, it is desirable to have a computer program that automatically provides the symmetry operations. In this paper, an approach is proposed for the derivation of symmetry operations from the $(3 + 1)$-dimensional superspace-group symbols (the two-line symbols). Based on this, a computer program *SPGR4D* has been written, which can easily be incorporated into other program packages. In fact, it has already been incorporated into the new version of the program *DIMS*.

2. Theoretical background

According to de Wolff (1974), a one-dimensional incommensurate crystal structure is represented by the periodic structure defined in the direct sum space $V_S = V_\varepsilon \oplus V_I$ with basis ($\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$, $\mathbf{e}_4$), where $\mathbf{e}_4$ is the unit vector perpendicular to the three-dimensional physical space V_ε, while ($\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$) forms the basis of the basic lattice. A vector in V_S can be expressed as

$$\mathbf{X} = x\mathbf{a} + y\mathbf{b} + z\mathbf{c} + t\mathbf{e}_4. \tag{1}$$

Positional defined quantities now depend not only on $\mathbf{r} = x\mathbf{a} + y\mathbf{b} + z\mathbf{c}$ but also on t; for example, the electron density $\rho(\mathbf{r})$ now corresponds to $\rho'(\mathbf{r}, t)$ with $\rho'(\mathbf{r}, t = 0) = \rho(\mathbf{r})$. The superspace symmetry operation $G(g_E, g_I)$ has the form (de Wolff, Janssen & Janner, 1981):

$$g_E\mathbf{r} \rightarrow \mathbf{r}' = R_E\mathbf{r} + \mathbf{s} \tag{2}$$

$$g_I\mathbf{t} \rightarrow \mathbf{t}' = \varepsilon t + \delta - \mathbf{q}\cdot\mathbf{s} = \varepsilon t + \tau - \mathbf{q}_i\cdot\mathbf{s} \tag{3}$$

with

$$\tau = \delta - \mathbf{q}_r\cdot\mathbf{s} \quad \text{and} \quad \mathbf{q} = \mathbf{q}_r + \mathbf{q}_i. \tag{4}$$

Here, $(R_E, \mathbf{s})$ is a space-group operation in conventional three-dimensional space, with R_E standing for the rotation and $\mathbf{s}$ for the translation. $\varepsilon = \pm 1$ and δ is a parameter that is an integer for all translations. $\mathbf{q}$ is the modulation wave vector. τ is the intrinsic rational increment in t, which is the most convenient parameter for characterizing g_I in superspace-group symbols as well as for characterizing extinction. The combinations (R_E, ε) are restricted by the following relations (de Wolff, 1977):

$$\varepsilon\mathbf{q}_i - R_E\mathbf{q}_i = 0 \tag{5}$$

and

$$\varepsilon\mathbf{q}_r - R_E\mathbf{q}_r = \mathbf{n}^*, \tag{6}$$

where $\mathbf{q}_i$ and $\mathbf{q}_r$ are mutually perpendicular components of $\mathbf{q}$.

The coordinates of $\mathbf{q}_r$ are simple rational fractions with respect to the basis of the basic lattice, whereas those of $\mathbf{q}_i$ are irrational ones. $\mathbf{n}^*$ is a reciprocal vector of the basic lattice. Equation (4) poses a restriction on $\mathbf{q}$ also.

For one-dimensional incommensurate modulated structures, there exist 775 inequivalent groups (de Wolff, Janssen & Janner, 1981; Yamamoto, Janssen, Janner & de Wolff, 1985). Each of these is uniquely denoted by a two-line symbol, such as $A^{Ammm}_{1\,s\,\bar{1}}$. The upper line contains the Hermann–Mauguin symbol for the basic space group. Below each generator g_E of the symbol, there is the corresponding g_I indicated by the intrinsic parameters in the following way. If $\varepsilon = -1$, there is always an origin such that τ vanishes. Thus, g_I is indicated by $\bar{1}$. For $\varepsilon = 1$, τ is invariant under a change of origin, and its value is one of the following:

$$\begin{array}{lccccc} \tau = & 0 & \frac{1}{2} & \pm\frac{1}{3} & \pm\frac{1}{4} & \pm\frac{1}{6} \\ \text{Symbol} & 1 & s & t & q & h \end{array} . \tag{7}$$

The prefix is selected to denote the $\mathbf{q}_r$ vector [see equation (4.4) of de Wolff, Janssen & Janner (1981)].

The lattice of a periodic structure in direct sum space V_S spanned by (de Wolff, 1974)

$$\begin{aligned} \mathbf{a}_1 &= \mathbf{a} - q^x\mathbf{e}_4 \\ \mathbf{a}_2 &= \mathbf{b} - q^y\mathbf{e}_4 \\ \mathbf{a}_3 &= \mathbf{c} - q^z\mathbf{e}_4 \\ \mathbf{a}_4 &= \mathbf{e}_4 \end{aligned} \tag{8}$$

is left invariant by the group of orthogonal transformations (which may be called a superspace point group) associated with the superspace group. $(\mathbf{a}, \mathbf{b}, \mathbf{c}, \mathbf{e}_4)$ and $(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3, \mathbf{a}_4)$ are two sets of basis vectors in V_S. They are related by an invertable 4×4 matrix $\mathbf{T}$:

$$(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3, \mathbf{a}_4) = (\mathbf{a}, \mathbf{b}, \mathbf{c}, \mathbf{e}_4)\mathbf{T}, \tag{9}$$

where

$$\mathbf{T} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ -q^x & -q^y & -q^z & 1 \end{bmatrix}, \qquad \mathbf{T}^{-1} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ q^x & q^y & q^z & 1 \end{bmatrix}. \tag{10}$$

Thus, the superspace symmetry transformations with respect to the basis $(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3, \mathbf{a}_4)$ can be deduced from (2) and (3), which have the form (Janner, Janssen & de Wolff, 1983)

$$G(R|\mathbf{v})\mathbf{X} = \Gamma(R)\mathbf{X} + \mathbf{v}, \tag{11}$$

with

$$\Gamma(R) = \begin{bmatrix} (R_E) & 0 \\ \Gamma_M(R) & \varepsilon \end{bmatrix} \tag{12}$$

and

$$\mathbf{v} = \begin{bmatrix} \mathbf{s} \\ \delta \end{bmatrix}. \tag{13}$$

where

$$\begin{aligned} \Gamma_M(R) &= \sigma\Gamma(R_E) - \varepsilon\sigma \\ &= [\sigma_r\Gamma(R_E) - \varepsilon\sigma_r] + [\sigma_i\Gamma(R_E) - \varepsilon\sigma_i] \end{aligned} \tag{14}$$

and $\Gamma(R_E)$ is the 3×3 matrix of R_E. With the restriction

$$\sigma_i\Gamma(R_E) - \varepsilon\sigma_i = 0, \tag{15}$$

$\Gamma_M(R)$ can be written as

$$\Gamma_M(R) = \sigma_r\Gamma(R_E) - \varepsilon\sigma_r. \tag{16}$$

Here, σ is defined by

$$\begin{aligned} \sigma &= (q^x, q^y, q^z) \\ &= (q^x_r, q^y_r, q^z_r) + (q^x_i, q^y_i, q^z_i) \\ &= \sigma_r + \sigma_i. \end{aligned} \tag{17}$$

3. The approach

Superspace groups are denoted by a two-line symbol, which consists of three parts. The prefix represents the component $\mathbf{q}_r$ of the modulation wave vector $\mathbf{q}$, the upper line is the Hermann–Mauguin symbol of the basic space group and the bottom line indicates the component g_I of the superspace group symmetry operation $G(g_E, g_I)$. In this section, an approach is described for the derivation of $(3 + 1)$-dimensional superspace symmetry operations from the two-line symbol based on the concept of generators. As mentioned above, a superspace-group symmetry element consists of R_E, ε, s, τ and $\mathbf{q}$, from which the operation can be set up following (2) and (3) or following (11). A detailed investigation of the $(3 + 1)$-dimensional superspace groups led to the conclusion that symmetry operations of each of these groups can be completed from a set of generators $\{[\Gamma(R^\nu_E), \varepsilon^\nu, \mathbf{s}^\nu, \tau^\nu, \mathbf{q}]|\nu = 1, \text{NG}\}$. Here $\{[\Gamma(R^\nu_E), \mathbf{s}^\nu)|\nu = 1, \text{NG}\}$ forms the set of generators for the basic space group represented by the upper line. The procedure to obtain the generating sets is given below.

3.1. *Derivation of generators for the basic space group*

The Hermann–Mauguin space-group symbols can be regarded as symbols for a set of generators of the group (Mauguin, 1931). The notation components can be divided into two categories: (i) components that represent the type of generating operations (generators) that comprise the generating set mentioned above; (ii) components that serve as indicators for the mutual orientation of the related symmetry elements (Hermann, 1931). A detailed investigation of the conventional space groups has been given by Burzlaff & Zimmermann (1980). On the basis of their investigation, a computer program for the derivation of symmetry operations from the space-group symbols was constructed (Burzlaff & Hountas, 1982), which can be used to provide the set of generators $\{[\Gamma(R^\nu_E), \mathbf{s}^\nu)|\nu = 1, \text{NG}\}$ for the basic space group. Here $\Gamma(R^\nu_E)$ is a 3×3 rotation matrix, $\mathbf{s}^\nu$ is the corresponding translational part, while NG stands for the number of generators in the set. This generating set is the starting point for the derivation of superspace groups.

Table 1. *Examples showing the input format for space groups*

Space group	Input format
$P^{B2/b}_{s\ \bar{1}}$ (**c** unique)	`P[B 2/B]S -1`
$P^{A2/a}_{s\ \bar{1}}$ (**b** unique)	`P[A 2/A]S -1  :B`
B^{Pc2a}_{111} (**c** unique)	`B[P C 2 A]1 -1 -1`
C^{Pba2}_{111} (**b** unique)	`C[P B A 2]-1 1 -1  :B`
D^{P2cb}_{111} (**a** unique)	`A[P 2 C B]-1 -1 1  :A`

3.2. *Determination of* ε^v *in the generating set*

Equation (5) or equation (15) imposes a strong restriction on ε. It can be shown that, for a given Bravais class, ε in the combination (R_E, ε) is uniquely determined by R_E. For Bravais classes with $\sigma_i = (0, 0, \gamma)$, we have $\sigma_i \Gamma(R_E) = \Gamma_{33}(R_E)\sigma_i$, thus $\varepsilon = \Gamma_{33}(R_E)$. For Bravais classes with $\sigma_i = (\alpha, \beta, 0)$, $\sigma_i \Gamma(R_E) = \Gamma_{11}(R_E)\sigma_i = \Gamma_{22}(R_E)\sigma_i$, leading to $\varepsilon = \Gamma_{11}(R_E) = \Gamma_{22}(R_E)$. If $\sigma_i = (\alpha, \beta, \gamma)$, we have $\sigma_i \Gamma(R_E) = \Gamma_{33}(R_E)\sigma_i$, which occurs only in Bravais class $P^{P\bar{1}}_{1}$, thus $\varepsilon = \Gamma_{11}(R_E) = \Gamma_{22}(R_E) = \Gamma_{33}(R_E)$. For different settings in the cases of monoclinic and orthorhombic classes, the relations between ε and $\Gamma(R_E)$ in the combination (R_E, ε) can be easily deduced as above. A table of ε values in the combination (R_E, ε) for the 24 Bravais classes can be found in Appendix *A*.

3.3. *Setting up* τ^v *values*

The value of τ defined in (4) is called the intrinsic rational increment in t. It has the following properties (de Wolff, Janssen & Janner, 1981): if $\varepsilon = 1$, τ is invariant under a change of origin and always has one of the values in (7); if $\varepsilon = -1$, there is always an origin such that $\tau = 0$. On the basis of these properties, the values of τ^v in $\{[\Gamma(R_E^v), \varepsilon^v, \mathbf{s}^v, \tau^v, \mathbf{q})|v = 1, \mathrm{NG}\}$ can be assigned by interpretation of the bottom line as follows:

(i) If $\varepsilon^v = 1$, τ^v is assigned according to (7).

(ii) If $\varepsilon^v = -1$ and all $\varepsilon^\mu = 1$ $(\mu \neq v)$, then τ^v can be assigned to 0, which is associated with the origin being fixed in the fourth dimension. In some cases, however, other values may be preferred. For example, the superspace group $P^{P2/m}_{s\ \bar{1}}$ has two generators $[\Gamma(2_z),\ 1,\ 0,\ \tau(2_z, 1),\ (0, 0, \gamma)]$ and $[\Gamma(\bar{m}_z),\ -1,\ 0,\ \frac{1}{2},\ (0, 0, \gamma)]$. Here, $\tau(R_E, \varepsilon)$ indicates that τ is associated with the combination (R_E, ε). If $\tau(2_z, 1)$ is assigned to 0, then $\tau(\bar{1}, \bar{1}) = \frac{1}{2}$, whereas $\tau(2_z, 1) = \frac{1}{2}$ leads to $\tau(\bar{1}, \bar{1}) = 0$. The latter assignment is preferred.

```
SYMMETRY CLASS:      MONOCLINIC
 SUPERSPACE GROUP:      P[B 2/B]1 -1
 SYMMETRICAL OPERATION:      +(0 0 0 0  1/2 0 1/2 0)

   1  0  0  0  .00    -1  0  0  0  .00     1  0  0  0  .00    -1  0  0  0  .00
   0  1  0  0  .00     0 -1  0  0  .50     0  1  0  0  .50     0 -1  0  0  .00
   0  0  1  0  .00     0  0 -1  0  .00     0  0 -1  0  .00     0  0 -1  0  .00
   0  0  0  1  .00     0  0  0  1  .00     0  0  0 -1  .00     0  0  0 -1  .00


SYMMETRY CLASS:      ORTHORHOMBIC
 SUPERSPACE GROUP:      C[P M A A]1 -1 1 :A
 SYMMETRICAL OPERATION:

   1  0  0  0  .00    -1  0  0  0  .00     1  0  0  0  .50     1  0  0  0  .50
   0  1  0  0  .00     0 -1  0  0  .00     0 -1  0  0  .00     0  1  0  0  .00
   0  0 -1  0  .00     0  0  1  0  .00     0  0 -1  0  .00     0  0 -1  0  .00
   0  0  0  1  .00     0  0  0 -1  .00     0  0  0  1  .00     0  0  0 -1  .00

  -1  0  0  0  .50    -1  0  0  0  .50     1  0  0  0  .00    -1  0  0  0  .00
   0 -1  0  0  .00     0  1  0  0  .00     0 -1  0  0  .00     0 -1  0  0  .00
   0  0  1  0  .00     0  0 -1  0  .00     0  0 -1  0  .00     0  0 -1  0  .00
   0  0  0 -1  .00     0  0  0 -1  .00     0  0  0 -1  .00     0  0  0 -1  .00
```

Fig. 1. Part of the text file OUTPUT.DAT.

(iii) When dealing with a generating set having two elements and both the corresponding values of ε equal to -1, we must use caution. This only occurs when the superspace group corresponds to the point group $\begin{smallmatrix}2&2\\1&1\end{smallmatrix}\begin{bmatrix}2\\1\end{bmatrix}$, $\begin{bmatrix}4\\1\end{bmatrix}\begin{smallmatrix}2&2\\1&1\end{smallmatrix}$ or $\begin{bmatrix}6\\1\end{bmatrix}\begin{smallmatrix}2&2\\1&1\end{smallmatrix}$. In this case, the two $\begin{smallmatrix}2\\1\end{smallmatrix}$ operations are selected as generators, while the operation in the square brackets serves as the indicator. If the τ associated with the indicator is not equal to 0, then τ^1 and τ^2 in the generating set cannot be assigned to 0 simultaneously, or the set will not make this group. An appropriate way to overcome this difficulty is to assign the τ value of the indicator to one of the generators. A list of τ^v values assigned for use in the program *SPGR4D* is given in Appendix *B*.

3.4. *About* $\mathbf{q}$ *or* σ

Following the prefix notation (de Wolff, Janssen & Janner, 1981), the rational part $\mathbf{q}_r$ or σ_r of $\mathbf{q}$ can be easily obtained by interpretation of the prefix in the two-line symbol. The irrational fraction $\mathbf{q}_i$ or σ_i is not used when the superspace-group operations are constructed on the basis $(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3, \mathbf{a}_4)$. If, on the other hand, the operations are to be set up on the basis $(\mathbf{a}, \mathbf{b}, \mathbf{c}, \mathbf{e}_4)$, then $\mathbf{q}_i$ must be given.

Following the above scheme, the generators $\{[\Gamma(R_E^v), \varepsilon^v, \mathbf{s}^v, \tau^v, \mathbf{q})|v = 1, \mathrm{NG}\}$ can be set up for each of $(3 + 1)$-dimensional superspace groups.

4. Example

Consider the superspace group $W^{P4_2/nnm}_{q\ \bar{1}\ q\ s}$. The basic space group is $P4_2/nnm$. The generating set of the basic space group consists of *nnm*, which stand respectively for a glide plane perpendicular to the reference direction [001], a glide plane perpendicular to [100] and a mirror plane perpendicular to [110]. The screw axis 4_2 associated with the reference direction [001] serves as an indicator. Choice of the origin at the inverse centre gives the three generating operations:

$$n[001]\quad \begin{matrix}1&0&0&\frac{1}{2}\\0&1&0&\frac{1}{2}\\0&0&\bar{1}&0\end{matrix},$$

$$n[101]\quad \begin{matrix}\bar{1}&0&0&0\\0&1&0&\frac{1}{2}\\0&0&1&\frac{1}{2}\end{matrix}$$

and

$$m[1\bar{1}0]\quad \begin{matrix}0&1&0&\frac{1}{2}\\1&0&0&\frac{1}{2}\\0&0&1&0\end{matrix},$$

where the 3×3 matrix is the rotation part while the 3×1 matrix stands for the translation vector **s**. Values of ε^v combined with the above three operations are -1, 1 and 1 , respectively. The corresponding τ^v are assigned respectively to 0, $\frac{1}{4}$ and $\frac{1}{2}$ according to the bottom line. The prefix W indicates $\mathbf{q}_r = (\frac{1}{2}, \frac{1}{2}, 0)$. By (4), the three values of δ are calculated to be $\frac{1}{2}$, $\frac{1}{2}$ and 0. Then, $\Gamma_M(R)$ for each combination (R_E^v, ε^v) is calculated from (16). Thus, the three generating operations of this superspace group are set up as follows:

Table 2. *ε values in the combination* (R_E, ε) *for 24 Bravais classes*

Column 1 lists the numbers of the Bravais class. Column 2 lists the symbols of the Bravais class together with the components $(\alpha, \beta, \gamma) = (q_i^x, q_i^y, q_i^z)$ of the vector $\mathbf{q}_i$. Different settings for the monoclinic and orthorhombic classes are listed with (*a*), (*b*) and (*c*) denoting, respectively, the **a**, **b** and **c** unique settings. $\Gamma_{\mu\mu}$ stands for the μth row and μth column of the rotation matrix $\Gamma(R_E)$.

	Bravais class			ε value		
No.	(*c*)	(*a*)	(*b*)	(*c*)	(*a*)	(*b*)
1	$P^{P\bar{1}}_{\bar{1}}(\alpha\beta\gamma)$			Γ_{11}		
2	$[P^{2/m}_{\bar{1}\ 1}(\alpha\beta 0)$	$P^{P2/m}_{\bar{1}\ 1}(0\beta\gamma)$	$P^{P2/m}_{\bar{1}\ 1}(\alpha 0\gamma)$	Γ_{11}	Γ_{22}	Γ_{33}
3	$C^{P2/m}_{\bar{1}\ 1}(\alpha\beta 0)$	$A^{P2/m}_{\bar{1}\ 1}(0\beta\gamma)$	$B^{P2/m}_{\bar{1}\ 1}(\alpha 0\gamma)$	Γ_{11}	Γ_{22}	Γ_{33}
4	$P^{B2/m}_{\bar{1}\ 1}(\alpha\beta 0)$	$P^{C2/m}_{\bar{1}\ 1}(0\beta\gamma)$	$P^{A2/m}_{\bar{1}\ 1}(\alpha 0\gamma)$	Γ_{11}	Γ_{22}	Γ_{33}
5	$P^{P2/m}_{1\ \bar{1}}(00\gamma)$	$P^{P2/m}_{1\ \bar{1}}(\alpha 00)$	$P^{P2/m}_{1\ \bar{1}}(0\beta 0)$	Γ_{33}	Γ_{11}	Γ_{22}
6	$A^{P2/m}_{1\ \bar{1}}(00\gamma)$	$B^{P2/m}_{1\ \bar{1}}(\alpha 00)$	$C^{P2/m}_{1\ \bar{1}}(0\beta 0)$	Γ_{33}	Γ_{11}	Γ_{22}
7	$P^{B2/m}_{1\ \bar{1}}(00\gamma)$	$P^{C2/m}_{1\ \bar{1}}(\alpha 00)$	$P^{A2/m}_{1\ \bar{1}}(0\beta 0)$	Γ_{33}	Γ_{11}	Γ_{22}
8	$B^{2/m}_{1\ \bar{1}}(00\gamma)$	$C^{C2/m}_{1\ \bar{1}}(\alpha 00)$	$A^{A2/m}_{1\ \bar{1}}(0\beta 0)$	Γ_{33}	Γ_{11}	Γ_{22}
9	$P^{Pmmm}_{1\ 1\ \bar{1}}(00\gamma)$	$P^{Pmmm}_{\bar{1}\ 1\ 1}(\alpha 00)$	$P^{Pmmm}_{1\ \bar{1}\ 1}(0\beta 0)$	Γ_{33}	Γ_{11}	Γ_{22}
10	$B^{Pmmm}_{1\ 1\ \bar{1}}(00\gamma)$	$C^{Pmmm}_{\bar{1}\ 1\ 1}(\alpha 00)$	$A^{Pmmm}_{1\ \bar{1}\ 1}(0\beta 0)$	Γ_{33}	Γ_{11}	Γ_{22}
11	$W^{Pmmm}_{1\ 1\ \bar{1}}(00\gamma)$	$U^{Pmmm}_{\bar{1}\ 1\ 1}(\alpha 00)$	$V^{Pmmm}_{1\ \bar{1}\ 1}(0\beta 0)$	Γ_{33}	Γ_{11}	Γ_{22}
12	$P^{Immm}_{1\ 1\ \bar{1}}(00\gamma)$	$P^{Immm}_{\bar{1}\ 1\ 1}(\alpha 00)$	$P^{Immm}_{1\ \bar{1}\ 1}(0\beta 0)$	Γ_{33}	Γ_{11}	Γ_{22}
13	$P^{Cmmm}_{1\ 1\ \bar{1}}(00\gamma)$	$P^{Ammm}_{\bar{1}\ 1\ 1}(\alpha 00)$	$P^{Bmmm}_{1\ \bar{1}\ 1}(0\beta 0)$	Γ_{33}	Γ_{11}	Γ_{22}
14	$L^{Cmmm}_{1\ 1\ \bar{1}}(00\gamma)$	$M^{Ammm}_{\bar{1}\ 1\ 1}(\alpha 00)$	$N^{Bmmm}_{1\ \bar{1}\ 1}(0\beta 0)$	Γ_{33}	Γ_{11}	Γ_{22}
15	$P^{Ammm}_{1\ 1\ \bar{1}}(00\gamma)$	$P^{Bmmm}_{\bar{1}\ 1\ 1}(\alpha 00)$	$P^{Cmmm}_{1\ \bar{1}\ 1}(0\beta 0)$	Γ_{33}	Γ_{11}	Γ_{22}
16	$A^{Ammm}_{1\ 1\ \bar{1}}(00\gamma)$	$B^{Bmmm}_{\bar{1}\ 1\ 1}(\alpha 00)$	$C^{Cmmm}_{1\ \bar{1}\ 1}(0\beta 0)$	Γ_{33}	Γ_{11}	Γ_{22}
17	$P^{Fmmm}_{1\ 1\ \bar{1}}(00\gamma)$	$P^{Fmmm}_{\bar{1}\ 1\ 1}(\alpha 00)$	$P^{Fmmm}_{1\ \bar{1}\ 1}(0\beta 0)$	Γ_{33}	Γ_{11}	Γ_{22}
18	$L^{Fmmm}_{1\ 1\ \bar{1}}(00\gamma)$	$M^{Fmmm}_{\bar{1}\ 1\ 1}(\alpha 00)$	$N^{Fmmm}_{1\ \bar{1}\ 1}(0\beta 0)$	Γ_{33}	Γ_{11}	Γ_{22}
19	$P^{P4/mmm}_{1\ \bar{1}\ 1\ 1}(00\gamma)$			Γ_{33}		
20	$W^{P4/mmm}_{1\ \bar{1}\ 1\ 1}(00\gamma)$			Γ_{33}		
21	$P^{I4/mmm}_{1\ \bar{1}\ 1\ 1}(00\gamma)$			Γ_{33}		
22	$P^{R\bar{3}m}_{\bar{1}\ 1}(00\gamma)$			Γ_{33}		
23	$R^{R\bar{3}m}_{\bar{1}\ 1\ 1}(00\gamma)$			Γ_{33}		
24	$P^{P6/mmm}_{1\ \bar{1}\ 1\ 1}(00\gamma)$			Γ_{33}		

Table 3. τ^v *values assigned for use in the program SPGR-4D*

Point group	Bottom line in the two-line symbol			τ^v		
1	1			0		
$\bar{1}$	$\bar{1}$			0		
2	$\bar{1}$			0		
	1			0		
	s			$\frac{1}{2}$		
m	$\bar{1}$			0		
	1			0		
	s			$\frac{1}{2}$		
$2/m$	$\bar{1}$	1		0	0	
	$\bar{1}$	s		$\frac{1}{2}$	$\frac{1}{2}$	
	1	$\bar{1}$		0	0	
	s	$\bar{1}$		$\frac{1}{2}$	$\frac{1}{2}$	
22(2)	$\bar{1}$	$\bar{1}$	(1)	0	0	
	$\bar{1}$	$\bar{1}$	(s)	0	$\frac{1}{2}$	
mm(2)	1	1	(1)	0	0	
	s	1	(s)	$\frac{1}{2}$	0	
	s	s	(1)	$\frac{1}{2}$	$\frac{1}{2}$	
	1	s	(s)	0	$\frac{1}{2}$	
	q	q	(1)	$\frac{1}{4}$	$\frac{1}{4}$	
m(2)m	1	($\bar{1}$)	$\bar{1}$	0	0	
	s	($\bar{1}$)	$\bar{1}$	$\frac{1}{2}$	0	
(2)mm	($\bar{1}$)	1	$\bar{1}$	0	0	
	($\bar{1}$)	s	$\bar{1}$	$\frac{1}{2}$	$\frac{1}{2}$	
	($\bar{1}$)	q	$\bar{1}$	$\frac{1}{4}$	$\frac{1}{4}$	
mmm	1	1	$\bar{1}$	0	0	0
	s	1	$\bar{1}$	$\frac{1}{2}$	0	$\frac{1}{2}$
	s	s	$\bar{1}$	$\frac{1}{2}$	$\frac{1}{2}$	0
	1	s	$\bar{1}$	0	$\frac{1}{2}$	$\frac{1}{2}$
	q	q	$\bar{1}$	$\frac{1}{4}$	$\frac{1}{4}$	0
4	1			0		
	s			$\frac{1}{2}$		
	q			$\frac{1}{4}$		
$\bar{4}$	$\bar{1}$			0		
$4/m$	1	$\bar{1}$		0	0	
	s	$\bar{1}$		$\frac{1}{2}$	0	
	q	$\bar{1}$		$\frac{1}{4}$	0	
(4)22	(1)	$\bar{1}$	$\bar{1}$	0	0	
	(s)	$\bar{1}$	$\bar{1}$	0	$\frac{1}{2}$	
	(q)	$\bar{1}$	$\bar{1}$	0	$\frac{1}{4}$	
(4)mm	(1)	1	1	0	0	
	(s)	s	1	$\frac{1}{2}$	0	
	(1)	s	s	$\frac{1}{2}$	$\frac{1}{2}$	
	(s)	1	s	0	$\frac{1}{2}$	
	(q)	q	1	$\frac{1}{4}$	0	
	(q)	q	s	$\frac{1}{4}$	$\frac{1}{2}$	
($\bar{4}$)m2	($\bar{1}$)	1	$\bar{1}$	0	0	
	($\bar{1}$)	s	$\bar{1}$	$\frac{1}{2}$	$\frac{1}{2}$	
	($\bar{1}$)	q	$\bar{1}$	$\frac{1}{4}$	0	
($\bar{4}$)2m	($\bar{1}$)	$\bar{1}$	1	0	0	
	($\bar{1}$)	$\bar{1}$	s	$\frac{1}{2}$	$\frac{1}{2}$	

Point group	Bottom line in the two-line symbol				τ^v		
(4)/mm	(1)	$\bar{1}$	1	1	0	0	0
	(s)	$\bar{1}$	s	1	0	$\frac{1}{2}$	0
	(1)	$\bar{1}$	s	s	0	$\frac{1}{2}$	$\frac{1}{2}$
	(s)	$\bar{1}$	1	s	0	0	$\frac{1}{2}$
	(q)	$\bar{1}$	q	1	0	$\frac{1}{4}$	0
	(q)	$\bar{1}$	q	s	0	$\frac{1}{4}$	$\frac{1}{2}$
3	1				0		
	t				$\frac{1}{3}$		
$\bar{3}$	$\bar{1}$				0		
32	1	$\bar{1}$			0	0	
	t	$\bar{1}$			$\frac{1}{3}$	0	
$3m$	1	1			0	0	
	1	s			0	$\frac{1}{2}$	
$\bar{3}m$	$\bar{1}$	1			0	0	
	$\bar{1}$	s			0	$\frac{1}{2}$	
3(1)2	1	(1)	$\bar{1}$		0	0	
	t	(1)	$\bar{1}$		$\frac{1}{3}$	0	
32(1)	1	$\bar{1}$	(1)		0	0	
	t	$\bar{1}$	(1)		$\frac{1}{3}$	0	
$3m$(1)	1	1	(1)		0	0	
	1	s	(1)		0	$\frac{1}{2}$	
3(1)m	1	(1)	1		0	0	
	1	(1)	s		0	$\frac{1}{2}$	
$\bar{3}$(1)m	$\bar{1}$	(1)	1		0	0	
	$\bar{1}$	(1)	s		0	$\frac{1}{2}$	
$\bar{3}m$(1)	$\bar{1}$	1	(1)		0	0	
	$\bar{1}$	s	(1)		0	$\frac{1}{2}$	
6	1				0		
	s				$\frac{1}{2}$		
	t				$\frac{1}{3}$		
	h				$\frac{1}{6}$		
$\bar{6}$	$\bar{1}$				0		
$6/m$	1	$\bar{1}$			0	0	
	s	$\bar{1}$			$\frac{1}{2}$	0	
(6)22	(1)	$\bar{1}$	$\bar{1}$		0	0	
	(s)	$\bar{1}$	$\bar{1}$		0	$\frac{1}{2}$	
	(t)	$\bar{1}$	$\bar{1}$		0	$\frac{1}{3}$	
	(h)	$\bar{1}$	$\bar{1}$		0	$\frac{1}{6}$	
(6)mm	(1)	1	1		0	0	
	(s)	s	1		$\frac{1}{2}$	0	
	(1)	s	s		$\frac{1}{2}$	$\frac{1}{2}$	
	(s)	1	s		0	$\frac{1}{2}$	
($\bar{6}$)m2	($\bar{1}$)	1	$\bar{1}$		0	0	
	($\bar{1}$)	s	$\bar{1}$		$\frac{1}{2}$	0	
($\bar{6}$)2m	($\bar{1}$)	$\bar{1}$	1		0	0	
	($\bar{1}$)	$\bar{1}$	s		0	$\frac{1}{2}$	
(6)/mmm	(1)	$\bar{1}$	1	1	0	0	0
	(s)	$\bar{1}$	s	1	0	$\frac{1}{2}$	0
	(1)	$\bar{1}$	s	s	0	$\frac{1}{2}$	$\frac{1}{2}$
	(s)	$\bar{1}$	1	s	0	0	$\frac{1}{2}$

$$\begin{array}{cccc} 1 & 0 & 0 & 0 & \frac{1}{2} \\ 0 & 1 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & \bar{1} & 0 & 0' \\ 1 & 1 & 0 & \bar{1} & \frac{1}{2} \end{array}$$

$$\begin{array}{cccc} \bar{1} & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 1 & 0 & \frac{1}{2} \\ \bar{1} & 0 & 0 & 1 & \frac{1}{2} \end{array}$$

and

$$\begin{array}{cccc} 0 & 1 & 0 & 0 & \frac{1}{2} \\ 1 & 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 1 & 0 & 0' \\ 0 & 0 & 0 & 1 & 0 \end{array}$$

from which all the other 13 symmetry operations can be derived.

5. The program

The program *SPGR4D* is written in Fortran77 and designed as a subroutine that is easily called by other programs. *SPGR4D* derives generators associated with the basis ($\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$, $\mathbf{a}_4$) according to a two-line superspace-group symbol input by the user. The program divides the superspace-group symbol into three parts: the prefix, the upper line and the bottom line. The program by Burzlaff & Hountas (1982) is incorporated into *SPGR4D* for the interpretation of the upper line. If the whole input symbol is one of the 230 conventional space groups, then *SPGR4D* (actually the program of Burzlaff & Hountas, 1982) will work out the generators in three-dimensional space. *SPGR4D* produces a complete set of symmetry operations. The rotational parts, $\Gamma(R)$ in (11), are stored in the integer array ROT(48, 4, 4). Translational parts are in the integer array TSL(48, 4). Components of $\mathbf{v}$ in (11) are obtained from TSL(48, 4) modulo 24. Basic translations associated with the centring of the lattice are stored in the integer TCL(4, 4) in the same way as that in TSL(48, 4). All the results, transformation matrices and basic translations are written to an output text file. It is assumed that the input information consists of the correct two-line symbols defined by de Wolff, Janssen & Janner (1981). No full control for internal consistency is performed. However, *SPGR4D* undertakes some checking on the bottom line. For example, W^{Pban}_{q1q} will be checked as an incorrect symbol and the user will be asked for a correction. For monoclinic and orthorhombic superspace groups, the default setting is assumed as **c** unique. Nonstandard settings should be declared with a note (:A for **a** unique and :B for **b** unique) next to the symbol. The input format of a two-line symbol is:

prefix [3D space-group symbol] bottom-line note,

in which the format of '3D (three-dimensional) space-group symbol' is the same as that used by Burzlaff & Hountas (1982). Some examples are given in Table 1. A simple program for calling *SPGR4D* is listed in Appendix *C*. With the input file INPUT.DAT containing a list of the 1997 (3 + 1)-dimensional superspace-group symbols, the program produces a full list of symmetry generators for all these space groups in 2 min when running on an IBM 386/33-compatible personal computer. The results are written to a text file OUTPUT.DAT, part of which is shown in Fig. 1.

APPENDIX *A*

Table 2 shows the ε values in the combination (R_E, ε) for 24 Bravais classes.

APPENDIX *B*

Table 3 shows the τ^v values assigned for use in the program *SPGR4D*.

APPENDIX *C*
A simple program calling the subroutine *SPGR4D*

```
C     MAIN
      INTEGER ERR,SYMBOL(80),ROT(48,4,4),TSL(48,4),TCL(4,4)
      OPEN(1,FILE='INPUT.DAT',STATUS='OLD')
      OPEN(2,FILE='OUTPUT.DAT',STATUS='UNKNOWN')
      DO 100 I=1,10000
      READ(1,'(80A1)',END=999) SYMBOL
      CALL SPGR4D(SYMBOL,ROT,TSL,TCL,NG,NLC,ERR,2,ICENT,I)
      IF(ERR.EQ.99) GOTO 999
100   CONTINUE
999   STOP
      END
```

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