

- HENDRICKSON, W. A. (1979). *Acta Cryst.* **A35**, 245–247.
 HENDRICKSON, W. A., KLIPPENSTEIN, G. L. & WARD, K. B. (1975). *Proc. Natl Acad. Sci. USA*, **72**, 2160–2164.
 HENDRICKSON, W. A., SMITH, J. L. & SHERIFF, S. (1985). *Methods Enzymol.* **115**, 41–55.
 JAMES, R. W. (1948). *The Optical Principles of the Diffraction of X-rays*. London: Bell & Sons.
 KRAUT, J. (1968). *J. Mol. Biol.* **35**, 511–512.
 OKAYA, Y. & PEPINSKY, R. (1956). *Phys. Rev.* **103**, 1645–1647.
 SHERIFF, S. & HENDRICKSON, W. A. (1987a). *Acta Cryst.* **A43**, 118–121.
 SHERIFF, S. & HENDRICKSON, W. A. (1987b). *Acta Cryst. B*. In the press.

Acta Cryst. (1987). **A43**, 125–130

A Real-Space Computer-Based Symmetry Algebra

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(Received 1 August 1985; accepted 3 September 1986)

Abstract

A computer-based symmetry algebra is described which permits the reconstruction of an infinite bond network from the asymmetric connectivity without an *a priori* knowledge of atomic coordinates. The algebra requires not only an algorithmic ordering of the Wyckoff groups but the designation of one site in each Wyckoff group as a special-position representative (SPR) site. The algebra is designed to be used for analysing the bonding network of compounds appearing in the Inorganic Crystal Structure Database.

Introduction

With the advent of crystal structure databases, computers are now used for the systematic examination of the structures of large numbers of related compounds. The program *SINDBAD* (Altermatt & Brown, 1985) has been used to calculate the bond vectors in the asymmetric unit from the atomic coordinates obtained from the Inorganic Crystal Structure Database (Bergerhoff, Hundt, Sievers & Brown, 1983). A systematic application of *SINDBAD* to entries stored in this database has resulted in the creation of a file (BONDFILE) containing the asymmetric bond sets of several thousand compounds. To expand the asymmetric set of bonds into the full bonding network requires the application of the symmetry operations of the appropriate space group. This can be done by computer, provided that proper care is taken in treating the bonds formed by atoms on special positions. This paper describes an algebra for doing this which, *inter alia*, requires an algorithm for

ordering the special positions and their representative sites.

Expansion of an asymmetric bond set

The BONDFILE contains the asymmetric set of bond vectors, each bond being identified by its two terminal atoms. Because of space limitations the atomic coordinates are not stored in the file. The asymmetric set of bond vectors is expanded into the full bond network by generating all the bonds around each of the terminal atoms of the network in turn. Each atom is identified by an index indicating which symmetry operator and which lattice vector is used to generate it from the given atom in the asymmetric unit. This index consists of five numbers, the first referring to an ordered list of atoms in the asymmetric unit, the second to an ordered list of symmetry operators, and the last three numbers to the lattice translation vector. The ordered list of symmetry operators could be a list of Seitz matrices which is stored explicitly in the BONDFILE, but we have found it more convenient to regenerate this list as required from the space-group symbol. Several programs are available to do this. The older ones interpret the Hermann–Mauguin symbol but recently new space-group symbols have been proposed (Hall, 1981; Shmueli, 1984) that are specifically designed to avoid the setting ambiguities inherent in the Hermann–Mauguin symbol. We have chosen to use the Hall (1981) symbol and the ordering of symmetry operators produced by the program *SGNAME* in *XTAL* (Stewart & Hall, 1983). This ordering is symbol dependent (it is even different for different symbols describing the same space-group setting), but since the Hall symbol that was used to generate the asymmetric set of bonds is the one stored in the BONDFILE, the program can always reconstruct the ordered list of symmetry operators appropriate to the problem.

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Treatment of atoms on special positions

If all atoms are on general positions, the expansion of the asymmetric set of bonds to the full network presents few difficulties, but to generate the bonds around an atom on a special position requires a knowledge of both the point group of the special position and its orientation. Although each Wyckoff group is associated with a unique point group, the point group may have different orientations at different sites. For example, in a tetragonal space group an atom on a (100) mirror plane will be related by the fourfold axis to another on a (010) mirror plane. An oriented point-group symbol could be stored for each atom in the network, but again it is more convenient to let the computer calculate it. It is, however, essential that the orientation of the point group of the atom in the asymmetric unit be known, and this can be ensured by defining one particular site in a Wyckoff group as a special-position representative (SPR) site. The asymmetric set of atoms is then chosen so that all the atoms occupy SPR sites. It is then necessary only to identify the Wyckoff group to which each atom belongs, and this can be done by reference to an ordered list of Wyckoff groups. The oriented point-group symbol of any atom in the crystal is found by applying the appropriate symmetry operator to the point-group symbol of the SPR for that atom. This formalism requires that the computer be able to generate an ordered list of Wyckoff groups for each space group and that it be able to determine the SPR site for each. An obvious choice of ordering would be that used in *International Tables for Crystallography* (1983), but unfortunately this cannot be used for several reasons, the chief being that any algorithmic ordering has to be setting dependent and the Wyckoff symbols are deliberately chosen to be setting independent. We have therefore devised our own ordering (Table 3) of the Wyckoff groups and we have defined an algorithm for determining which site in a Wyckoff group is the SPR (Table 2). Although our ordering, being necessarily setting dependent, cannot always reproduce that used in *International Tables for Crystallography*, we have preserved the principle of ordering on the degree of symmetry by sorting first on the site multiplicity. Our first Wyckoff group is always the general position, a choice which has some obvious programming advantages. The second sort can be based either on the point group (which would bring together Wyckoff groups of similar symmetry) or on the coordinates of the SPR. We have chosen the latter sorting because the point-group symbol may not always be available since there are many applications in which it is not needed. In any case, since the symmetry is treated entirely within the program, the user does not need to be aware of the ordering or even of the existence of special positions. Should the user particularly want to examine

Table 1. Example of the use of the Seitz-matrix formalism, the special-position representative and the special-position symmetry table

Space group	$P2_1/m$		
Symmetry operators:	$x, y, z \quad -x, \frac{1}{2}+y, -z \quad -x, -y, -z \quad x, \frac{1}{2}-y, z$		
which are represented as (S/T) :			
(1)	1 0 0 0-0	(2)	-1 0 0 0-0
	0 1 0 0-0		0 1 0 0-5
	0 0 1 0-0		0 0 -1 0-0
(3)	-1 0 0 0-0	(4)	1 0 0 0-0
	0 -1 0 0-0		0 -1 0 0-5
	0 0 -1 0-0		0 0 1 0-0

The special-position representative is for

site 2(e) ($k=2$):	site 2(d) ($k=3$):
$(x, \frac{1}{4}, z)$	$(\frac{1}{2}, 0, \frac{1}{2})$
$(SP/TP)_{2r}$	$(SP/TP)_{3r}$
1 0 0 0-0	0 0 0 0-5
0 0 0 0-25	0 0 0 0-0
0 0 1 0-0	0 0 0 0-5

The special-position symmetry table in the form $i(j)_k$ for $(SP/TP)_{ki} = (S/T)_j * (SP/TP)_{kr}$, for the above two positions is

$j (= i_1) =$	1 2 3 4
$i_2 =$	1 2 2 1
$i_3 =$	1 2 1 2.

the special positions and their ordering our program *GETSPEC* described in the Appendix can produce a listing in the *International Tables for Crystallography* format.

Symmetry representation and handling in computer programs

A simple way to store symmetry operators in a computer program is in the form of Seitz matrices (S/T) (Seitz, 1936; Bradley & Cracknell, 1972). These are 4×4 matrices which can be decomposed into a rotational 3×3 matrix S and a translational 3-vector T . The Seitz-matrix formulation can also be used for representing special position operators (SP/TP) , allowing one to specify the particular free (SP) and fixed (TP) coordinates of the site (see Table 1 for an example). For each Wyckoff group or special position k a set of operators $\{(SP/TP)_{kj}, j=1, m_k\}$; where $m_k =$ group multiplicity is defined which transforms an arbitrary coordinate vector $X_a = (x, y, z)^\dagger$ to the set of coordinate vectors $\{X_{akj}, j=1, m_k\}$ which define all possible sites of the k th Wyckoff group within the primitive unit cell:

$$X_{akj} = (SP/TP)_{kj} * X_a. \quad (1)$$

Only the special-position representative operator, $(SP/TP)_{kr, \ddagger}$ is needed to define the Wyckoff group

[†] Note that in general one or more of the coordinates x, y and z will be undefined and can be set to any value. However, in order for equation (6) (below) to hold, they should be given the actual coordinates required by the SPR.

[‡] The way in which $(SP/TP)_{kr}$ is chosen is described below.

k , because all the other sites can be found using

$$\begin{aligned} \mathbf{X}_{akj} &= (S/T)_j * (SP/TP)_{kr} * \mathbf{X}_a \\ &= \mathbf{S}_j * \mathbf{SP}_{kr} * \mathbf{X}_a + \mathbf{S}_j * \mathbf{TP}_{kr} + \mathbf{T}_j \end{aligned} \quad (2)$$

or

$$(SP/TP)_{kj} = (S/T)_j * (SP/TP)_{kr}. \quad (3)$$

However, applying (3) using all values of j will, in general, create the set $\{\mathbf{X}_{akj}\}$ several times depending on the multiplicity m_k of the Wyckoff position. It is therefore necessary to set up a special-position symmetry (SPS) table which indicates which symmetry operators acting on the SPR give identical special-position operators. Table 1 gives an example. All the information about the point group of the SPR and its orientation is contained in the SPS table.

The formalism described above gives only the transformations produced by the set of primitive symmetry operators [those listed in *International Tables for Crystallography* (1983)]. In order to generate atoms in any desired part of the crystal we expand the Seitz matrix by the addition of a lattice vector \mathbf{L}_l . The set of symmetry and translation operators $\{(S/T)_j L_l\}$ is infinite for an unbounded crystal and includes all possible symmetry operations within the crystal. The transformation of an arbitrary position, \mathbf{X}_a , to a symmetry-dependent one anywhere else in the crystal becomes

$$\mathbf{X}_{ajl} = (S/T)_j L_l * \mathbf{X}_a = \mathbf{S}_j * \mathbf{X}_a + \mathbf{T}_j + \mathbf{L}_l, \quad (4)$$

and for a special position k the transformation becomes

$$\begin{aligned} \mathbf{X}_{akjl} &= (S/T)_j L_l * (SP/TP/LP)_{kr} * \mathbf{X}_a \\ &= \mathbf{S}_j * \mathbf{SP}_{kr} * \mathbf{X}_a + \mathbf{S}_j * (\mathbf{TP}_{kr} + \mathbf{LP}_{kr}) + \mathbf{T}_j + \mathbf{L}_l \end{aligned} \quad (5)$$

where the special-position representative $(SP/TP/LP)_{kr}$ can always be chosen so that \mathbf{LP}_{kr} is a zero vector. The notation $(SP/TP)_{kr}$ is therefore quite general.

The above formalism allows one to manipulate the symmetry operators without reference to the actual value of the coordinates \mathbf{X}_a of the atom \mathbf{a} in the asymmetric unit provided that the values of \mathbf{X}_a are those of the SPR. This is fulfilled when

$$\mathbf{X}_a = (SP/TP)_{kr} * \mathbf{X}_a. \quad (6)$$

This restriction is essential since the symmetry operator $(S/T)_i L_l$ that transforms a special-position operator into itself,

$$(SP/TP)_{kj} = (S/T)_i L_l * (SP/TP)_{kj}, \quad (7)$$

will in general be different for different values of j . It is therefore necessary to start with an identified member of the set $\{(SP/TP)_{kj}, j = 1, m_k\}$, namely the SPR. The general position is treated in the same way

as a special position, but since in this case $\mathbf{SP} = \mathbf{l}$ and $\mathbf{TP} = \mathbf{0}$, there are no restrictions on the choice of the coordinates \mathbf{X}_a . The coordinates of any atom in the crystal are then given as

$$\mathbf{X}_{akjl} = (S/T)_j L_l * (SP/TP)_{kr} * \mathbf{X}_a. \quad (8)$$

Since the symmetry transformation is defined uniquely by the indices k, j and l , they can be manipulated without any direct knowledge of \mathbf{X}_a . The index k can be found by reference to a table of properties of the atom a , so that it need not be given explicitly, leaving only the five integers a, j and l (3) to identify uniquely each atom in the crystal. The converse is not true since there are always at least two ways of generating the coordinates of an atom on a special position. In order to ensure that the index for each atom is also unique it is necessary to specify which symmetry operator is to be used in cases where there is a choice. This information is stored in the SPS table.

Treatment of interatomic distances

Interatomic distances can be defined in terms of a vector \mathbf{V}_b ($\mathbf{V}_b = \mathbf{X}_{a_2 j_2 l_2} - \mathbf{X}_{a_1 j_1 l_1}$) between the two atoms a_1, j_1, l_1 and a_2, j_2, l_2 . The complete set of symmetry-equivalent distances can be generated by application of the symmetry operations $(S/T)_j L_l$ resulting in the vector

$$\mathbf{V}_{bj'} = \mathbf{S}_{j'} * \mathbf{V}_b \quad (9)$$

between the atoms a_1, j_1', l_1' and a_2, j_2', l_2' , where

$$\mathbf{X}_{aj'l'} = (S/T)_{j'} L_{l'} * \mathbf{X}_{ajl}. \quad (10)$$

In particular it is possible to generate all the symmetry-equivalent distances around an atom (a_1, j_1, l_1) on a special position by applying those symmetry operations (as given in the SPS table) that leave the indices of this atom invariant. It is therefore not even necessary to know the distance vector \mathbf{V} that describes a bond in order to reconstruct the complete connectivity within a crystal; it is sufficient to know the indices of the atoms that define the asymmetric set of bonds.

Calculation of the special-position operators

In order to calculate the special-position operators (SP/TP) it is first necessary to generate the symmetry operators (S/T) . We have written a Fortran program based on the algorithm used in *XTAL* (Stewart & Hall, 1983) to calculate an ordered list of primitive symmetry operators (those not involving lattice translations) from the Hall space-group symbol (Hall, 1981). These operators are used to generate the SPR, $(SP/TP)_{kr}$, for each of the special positions of the space group as described below. At the same time our program calculates the SPS table for each SPR.

It is written in the form of the list $i(j)_k$ in which i is the symmetry operator with the lowest index that is equivalent to j for the particular SPR. An example of an SPS table is given in Table 1.

Selection of the special-position representative

Since the ordering of the special positions involves the coordinates of the special-position representatives (SPR), it is first necessary to describe how these are defined for a given Wyckoff group k . We first calculate all elements of the Wyckoff group in the primitive cell, add all possible lattice translations to adjacent cells and then redefine the independent parameters in the rotational part of the Seitz matrix so that in the vector $\mathbf{X}_{kj} [= (x_s, y_s, z_s) = (SP/TP)_{kj} * \mathbf{X}_a]$, if x_s is dependent on y or z , the independent variable is relabelled as x and if there is a dependent variable it is chosen to be z_s .

As an example, consider the tetragonal space group in which the special position k contains

$$\mathbf{X}_{k1} = \left(\frac{3}{4}, y, z\right) \quad \text{as} \quad (SP/TP)_{k1} = \begin{matrix} 0 & 0 & 0 & 0.75 \\ 0 & 1 & 0 & 0.0 \\ 0 & 0 & 1 & 0.0 \end{matrix}$$

and

$$\mathbf{X}_{k2} = \left(y, \frac{1}{4}, z\right) \quad \text{as} \quad (SP/TP)_{k2} = \begin{matrix} 0 & 1 & 0 & 0.0 \\ 0 & 0 & 0 & 0.25 \\ 0 & 0 & 1 & 0.0 \end{matrix}$$

This redefinition leads to

$$(SP/TP)_{k1} = \begin{matrix} 0 & 0 & 0 & 0.75 \\ 1 & 0 & 0 & 0.0 \\ 0 & 0 & 1 & 0.0 \end{matrix} \quad \text{or} \quad \mathbf{X}_{k1} = \left(\frac{3}{4}, x, z\right)$$

and

$$(SP/TP)_{k2} = \begin{matrix} 1 & 0 & 0 & 0.0 \\ 0 & 0 & 0 & 0.25 \\ 0 & 0 & 1 & 0.0 \end{matrix} \quad \text{or} \quad \mathbf{X}_{k2} = \left(x, \frac{1}{4}, z\right).$$

The fourteen steps listed in Table 2 are then applied. They are designed to select the SPR as the Seitz matrix with the fewest and most positive elements in the rotational part (SP) and the smallest overall translation (TP).

Ordering the special positions

The sorting of the SPR's to produce an ordered list of all special positions k is based first on the site multiplicity, then on the number of independent and dependent coordinates, and finally on the number of fixed coordinates and the sum of their values as described in Table 3. The general position is always

Table 2. Steps taken to select the SPR as the Seitz matrix with fewest and most positive elements in the rotational part and smallest overall translation

In a special position k given by the set of Seitz matrices $\{(SP/TP)_{kj}, j=1, \text{multiplicity}\}$ apply the following tests in the order given to select the special-position representative $(SP/TP)_{k_r}$. At each test reject all unselected elements of $\{(SP/TP)_{kj}\}$ until only the one representative is left.

Representing the elements of $(SP/TP)_{kj}$ as $(sp_{um})/(tp_u)$; $u=1, 2, 3$, $m=1, 2, 3$, select the elements where:

- (1) if $SP = \text{zero matrix}$: TP has the fewest components and $\sum_u tp_u$ is minimum,
- (2) $sp_{11} \geq 0$, $sp_{12} = sp_{13} = 0$ and SP has the fewest non-zero diagonal elements sp_{uu} ,
- (3) if sp_{uu} is non-zero: $tp_u = 0$,
- (4) $sp_{22} \geq 0$,
- (5) $sp_{23} = 0$,
- (6) tp_1 minimum,
- (7) $sp_{33} \geq 0$,
- (8) if $sp_{11} = 0$: $sp_{21} = 0$,
- (9) $sp_{21} \leq 1$,
- (10) $sp_{21} \geq 0$,
- (11) tp_2 minimum,
- (12) tp_3 minimum,
- (13) if $sp_{11} = 0$: $sp_{31} = 0$,
- (14) $sp_{3m} \geq 0$.

If there is no element left after a given test, the ones rejected in the current test are reset and the next test is applied. If after a given test only one (SP/TP) is left, this is the representative $(SP/TP)_{k_r}$ for the special position k .

Table 3. Sorting of the SPR's

To sort the special-position representatives of two Wyckoff groups, $(SP/TP)_{k_1,r}$ and $(SP/TP)_{k_2,r}$, in order, place higher in the list the one with:

- (1) the higher multiplicity;
- (2) more independent parameters (non-zero diagonal elements in SP);
- (3) more dependent parameters (non-zero off-diagonal elements in SP);
- (4) if there are two independent parameters: the one with $SP(3, 3) = 0$ and $TP(3)$ smaller, or $SP(2, 2) = 0$ and $TP(2)$ smaller, or $SP(1, 1) = 0$ and $TP(1)$ smaller, in that order;
- (5) if there is one independent parameter: $SP(3, 3) \neq 0$ and $TP(1)$ smaller [and/or $TP(2)$ smaller] or $SP(2, 2) \neq 0$ and $TP(1)$ smaller [and/or $TP(3)$ smaller] or $SP(1, 1) \neq 0$ and $TP(2)$ smaller [and/or $TP(3)$ smaller] in that order;
- (6) the large number of non-zero fixed parameters;
- (7) if there are two non-zero fixed parameters: $TP(3) = 0$ or $TP(2) = 0$ or $TP(1) = 0$ in that order;
- (8) if there is one non-zero fixed parameter: $TP(1) \neq 0$ or $TP(2) \neq 0$ or $TP(3) \neq 0$, in that order;
- (9) the larger sum $TP(1) + TP(2) + TP(3)$.

The tests are applied in the order given until a difference in the two representatives leads to an ordering. The representatives in the ordered list are then numbered from top to bottom, so that the first position (at the top of the list) is the general position (see Table 4).

included as the first Wyckoff group, and the last position in the list will therefore have the smallest possible multiplicity and have the fixed coordinates closest to the origin.

Table 4 gives an example and compares our sorted list of special positions with the corresponding list in *International Tables for Crystallography* (1983). In many cases the proposed sorting scheme leads to a list identical to the one in *International Tables*, but the sorting in *International Tables* is primarily based

Table 4. Comparison of sorted SPR list with that in *International Tables for Crystallography* (1983)Space group number 112, $P\bar{4}2c$.

In each listing the columns are

- | | |
|-----------------------------|-------------------------|
| 1. special position number, | 4. site point symmetry, |
| 2. multiplicity, | 5. coordinates. |
| 3. Wyckoff letter, | |

<i>International Tables</i> listing		Proposed listing	
1 8 n 1	x, y, z	1 8 n 1	x, y, z
2 4 m 2..	$0, \frac{1}{2}, z$	2 4 l 2..	$\frac{1}{2}, \frac{1}{2}, z$
3 4 l 2..	$\frac{1}{2}, \frac{1}{2}, z$	3 4 m 2..	$0, \frac{1}{2}, z$
4 4 k 2..	$0, 0, z$	4 4 k 2..	$0, 0, z$
5 4 j .2.	$0, y, \frac{1}{4}$	5 4 h .2.	$x, \frac{1}{2}, \frac{1}{4}$
6 4 i .2.	$x, \frac{1}{2}, \frac{1}{4}$	6 4 i .2.	$x, \frac{1}{2}, \frac{1}{4}$
7 4 h .2.	$\frac{1}{2}, y, \frac{1}{4}$	7 4 j .2.	$x, 0, \frac{1}{4}$
8 4 g .2.	$x, 0, \frac{1}{4}$	8 4 g .2.	$x, 0, \frac{1}{4}$
9 2 f -4..	$\frac{1}{2}, \frac{1}{2}, 0$	9 2 c 222.	$\frac{1}{2}, \frac{1}{2}, \frac{1}{4}$
10 2 e -4..	$0, 0, 0$	10 2 f -4..	$\frac{1}{2}, \frac{1}{2}, 0$
11 2 d 222.	$0, \frac{1}{2}, \frac{1}{4}$	11 2 b 222.	$\frac{1}{2}, 0, \frac{1}{4}$
12 2 c 222.	$\frac{1}{2}, \frac{1}{2}, \frac{1}{4}$	12 2 d 222.	$0, \frac{1}{2}, \frac{1}{4}$
13 2 b 222.	$\frac{1}{2}, 0, \frac{1}{4}$	13 2 a 222.	$0, 0, \frac{1}{4}$
14 2 a 222.	$0, 0, \frac{1}{4}$	14 2 e -4..	$0, 0, 0$

on the site symmetries whereas the present ordering is based on the coordinate representation.

Discussion

A program, *GETSPEC*, which incorporates these algorithms is described in the Appendix and is available from the authors. We have also written programs which use the above formalism to carry out an expansion of a bonded set of atoms. These include subroutines which perform basic operations with the indices. Among these are multiplication

$$(kj_3l_3) = (kj_2l_2) * (kj_1l_1)$$

and inverse multiplication

$$(kj_3l_3) = (kj_2l_2)^{-1} * (kj_1l_1).$$

In each case the value of j_3 is uniquely determined from the group multiplication table and the SPS table, whereas l_3 has to be calculated explicitly. We have also written routines to generate the atom indices corresponding to the set of operators (2) that are equivalent to a given operator (1) around the special position k :

$$(kj_2l_2) \equiv (kj_1l_1).$$

Our purpose in developing the symmetry handling procedures described above is to allow us to manipulate bonding networks by computer in such a way that the user does not have to be concerned with the details, or even the existence, of symmetry. As further applications of computers in crystal chemistry are developed there will be an increased need for algorithmic orderings of symmetry operators and special positions to supplement the descriptions given in *International Tables for Crystallography* (1983). The formalism given in this paper is designed to provide a basis for the further development of computer manipulation of crystallographic symmetry.

We thank the Natural Sciences and Engineering Research Council of Canada for an operating grant and Mr David Moss crop for coding the routine that calculates the symmetry operators.

APPENDIX

Program *GETSPEC*

Input/output

The only input needed is the Hall space-group symbol (Hall, 1981) but the program comes with a file containing the Hall symbols corresponding to the modified Hermann-Mauguin symbols used in the Inorganic Crystal Structure Database. The only restriction our program requires is that the unique hexagonal axis be the c axis.

The output of the program consists of the Seitz matrices of all the symmetry operators and, using a similar matrix representation, the special-position representative of each Wyckoff group, sorted according to the ordering scheme described in the paper. Special-position point-group symbols as described in *International Tables for Crystallography* (Hahn & Vos, 1983) are also created. The output is written in the Standard Crystallographic File Structure (SCFS) (Brown, 1985). Table 5 shows the SCFS output for a non-centrosymmetric setting of *Pbmn* (number 53) and Table 6 gives an example of the printed output.

Program structure

The calling program reads the space-group symbol and then calls the following subroutines:

- SPACRD* to transform a Hermann-Mauguin symbol to a Hall symbol using table look-up,
- SGHALL* to calculate the symmetry operators of the general position from the Hall symbol. This routine is based on *SGNAME* used in *XTAL* (Stewart & Hall, 1983),
- GRMULT* to calculate the group multiplication table,
- SPOST* to derive the special-position representative (SPR) site for each special position,
- SPESOR* to sort the special positions,
- SPMULT* to derive the special-position symmetry table,
- SPSYM* to create the special-position point-group symbol,
- WSCFS* to write the information on an SCFS file.

Finally the calling program prints an output listing in an easily readable form (Table 6).

All subroutines are written in machine-independent Fortran 77 and both VAX and Cyber versions are available for the calling program which also contains

Table 5. SCFS output for a non-centrosymmetric setting of *Pbmn*

SCFS output (*N.B.* this is a non-standard extension of SCFS-84. A standard SCFS-87 version will be available when the new version of SCFS is approved).

```
TITLE
* An example illustrating the SG OPERATORS section
SG NAME
HALL P 2A 2A-1B
*EOS
SYMMETRY (Format: A1, 2A4, 3(3I2, F10.7, 4X))
  1  0  0  0-0000000  0  1  0  0-0000000  0  0  1  0-0000000
 -1  0  0  0-5000000  0 -1  0  0-0000000  0  0  1  0-0000000
  1  0  0  0-5000000  0 -1  0  0-0000000  0  0 -1  0-0000000
 -1  0  0  0-0000000  0 -1  0  0-5000000  0  0 -1  0-0000000
 -1  0  0  0-0000000  0  1  0  0-0000000  0  0 -1  0-0000000
  1  0  0  0-5000000  0  1  0  0-5000000  0  0 -1  0-0000000
 -1  0  0  0-5000000  0  1  0  0-5000000  0  0  1  0-0000000
  1  0  0  0-0000000  0 -1  0  0-5000000  0  0  1  0-0000000
*EOS
SG OPERATORS (Format: A1, 2A4, 3(3I2, F10.7), I3, A1, 1X, A8)
SPEC  1  0  0  0-0000000  0  1  0  0-0000000  0  0  1  0-0000000  8  1
SPEC  1  0  0  0-0000000  0  0  0-2500000  0  0  1  0-0000000  8  .M.
SPEC  0  0  0  0-2500000  0  0  0-0000000  0  0  1  0-0000000  4  ..2
SPEC  0  0  0  0-0000000  0  1  0  0-0000000  0  0  0-2500000  4  .2.
SPEC  0  0  0  0-0000000  0  1  0  0-0000000  0  0  0-0000000  4  .2.
SPEC  0  0  0  0-0000000  0  0  0-7500000  0  0  0-5000000  2  .2/M.
SPEC  0  0  0  0-0000000  0  0  0-2500000  0  0  0-5000000  2  .2/M.
SPEC  0  0  0  0-0000000  0  0  0-7500000  0  0  0-0000000  2  .2/M.
SPEC  0  0  0  0-0000000  0  0  0-2500000  0  0  0-0000000  2  .2/M.
*EOS
END
```

enough information about the common block structures to allow the subroutines to be used independently in other program packages. *SPOST*, the heart of the program, contains about 1100 lines of Fortran code and comments; all routines together contain about 3500 lines. No overlay structure is necessary for the Cyber.

Algorithm

No general algorithm could be found for *SPOST* that would work for all symmetry operators in all crystallographic systems with no limits on the choice of axes. The program therefore runs through the entire set of symmetry operators trying to solve all equations of the type

$$I * X = S_i * X + T_i + L_j,$$

i.e.

$$X = (I - S_i)^{-1} * (T_i + L_j), \quad (A1)$$

where X is the positional vector representing the special position created by the i th symmetry operator (X generally has free and fixed components), I is the identity matrix, S_i is the rotation (3×3) matrix and T_i is the translation 3-vector associated with the i th symmetry operator, and L_j is any lattice translation vector. Only when the i th symmetry operator gives rise to a special position does (A1) have a solution.

The program recognizes the different forms of (A1) and explores and tests the possible solutions, X .

Table 6. Example of the printed output

Print output (note that this is non-standard setting indicated by the final letter of the Hermann-Mauguin symbol).

```
Space group nr. 53
Hermann-Mauguin symbol PBMNS
Hall symbol P 2A 2A-1B
Symmetry operators:
  1 +X, +Y, +Z
  2 1/2-X, -Y, +Z
  3 1/2+X, -Y, -Z
  4 -X, 1/2-Y, -Z
  5 -X, +Y, -Z
  6 1/2+X, 1/2+Y, -Z
  7 1/2-X, 1/2+Y, +Z
  8 +X, 1/2-Y, +Z
Listing of special position:
  Nr. coordinates multiplicity site symmetry
  1 X, Y, Z 8 1
  2 X, 1/4, Z 4 .M.
  3 1/4, 0, Z 4 ..2
  4 0, Y, 1/2 4 .2.
  5 0, Y, 0 4 .2.
  6 0, 3/4, 1/2 2 .2/M.
  7 0, 1/4, 1/2 2 .2/M.
  8 0, 3/4, 0 2 .2/M.
  9 0, 1/4, 0 2 .2/M.
Elapsed CPU time (VAX 780): 1.93 Seconds
```

Results

More than 490 different settings of the 230 space groups are found in the Inorganic Crystal Structure Database and all have been run through *GETSPEC* on a VAX 780 computer. For triclinic, monoclinic and orthorhombic space groups with less than three mirror planes the computing time needed is less than 1.2 s; orthorhombic *mm* groups, lower symmetry tetragonal and hexagonal space groups need up to 6 s; 4/*mmm* and 6 *mmm* groups may need up to 23 s. The cubic groups mostly run in less than 30 s, but space groups 221-230 need 55-330 s. We have not found any way to reduce the time required for these last ten space groups but we believe that users concerned only with highly symmetric cubic groups may be able to write a special program that will be much faster.

References

- ALTERMATT, D. & BROWN, I. D. (1985). *Acta Cryst.* **B41**, 240-244.
 BERGERHOFF, G., HUNDT, R., SIEVERS, R. & BROWN, I. D. (1983). *J. Chem. Inf. Comput. Sci.* **23**, 66-69.
 BRADLEY, C. J. & CRACKNELL, A. P. (1972). *The Mathematical Theory of Symmetry in Solids*. Oxford: Clarendon Press.
 BROWN, I. D. (1985). *Acta Cryst.* **A41**, 399.
 HAHN, TH. & VOS, A. (1983). *International Tables for Crystallography*, Vol. A, pp. 26-28. Dordrecht: Reidel.
 HALL, S. R. (1981). *Acta Cryst.* **A37**, 517-525.
International Tables for Crystallography (1983). Vol. A, edited by TH. HAHN. Dordrecht: Reidel.
 SEITZ, F. (1936). *Ann. Math.* **37**, 17-28.
 SHMUELI, U. (1984). *Acta Cryst.* **A40**, 559-567.
 STEWART, J. M. & HALL, S. R. (1983). *The XTAL System of Crystallographic Programs*. Univ. of Maryland.