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Space-Group Algorithms. I. The Space Group and Its Symmetry Elements

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Abstract

A well-defined and efficient algorithm, which enables the derivation of any crystallographic space group and full characterization of its symmetry operations and elements, is described and illustrated. The algorithm is based on a representation of crystallographic point groups in terms of cyclic groups, and on isomorphism relations between the point groups and the corresponding factor-group representations of the space groups. The characterization of the symmetry operations and the corresponding symmetry elements is also presented in an algorithmic manner, with particular emphasis on the orientation of the axes of rotation and their location vectors. The above algorithms have been implemented in a computer program, an application of which to the space group $Pa\bar{3}$ is shown and some relevant programming considerations are given. The input to this general program can be fully adapted to the space-group tables in Vol. A of *International Tables for Crystallography* [(1983). Dordrecht: Reidel].

Introduction

The merits of an automated derivation of space-group information become apparent when such information is routinely required on space groups of higher symmetry, or when crystal symmetry has to be regarded as a 'parameter' in theoretical considerations. Clearly, computer-generated symmetry information reduces the possibility of human error and may lead to most significantly increased efficiency of the calculations.

Algebraic formalisms, related to a systematic derivation of space groups, have long since been established (Seitz, 1934, 1935*a*, *b*; Zachariasen, 1967) and computational approaches to the various aspects of this topic were put forward (*e.g.* Wells, 1965; Wondratschek & Neubüser, 1967; Burzlaff & Zimmermann, 1980). Three relevant computer programs have recently been reported (Fokkema, 1975; Hall, 1981; Burzlaff & Hountas, 1982) and the first of these was used in the generation and production of the space-group tables in *International Tables for Crystallography* (1983), which will hereafter be referred to as ITA83.

The present author's interest in this subject arose in connection with studies of generalized intensity statistics, which required all-space-group calculations of absolute moments of the trigonometric structure factor (Shmueli & Wilson, 1981; Shmueli, 1982; Shmueli & Kaldor, 1981, 1983), by methods of symbolic programming. Obviously, computer-generated symmetry information and its automatic transfer to subsequent computations are of great value in such calculations, as well as in many other applications involving space-group symmetry.

After some preliminary experiments it was decided to base the algorithm on the method due to Zachariasen (1967), in which the following advantages seem to be apparent: (i) the generators are explicitly contained in the space-group symbol, which is therefore very easily decoded; (ii) Zachariasen's approach is simply related to basic group theory, it has a concise structure and provides relations that are to be satisfied by the generators; (iii) the sequence of the algebraic operations to be performed is exactly prescribed by the space-group symbol, thus avoiding any search for new operations; and (iv) the space-group symbols, proposed by Zachariasen (1967), can be easily adapted to programming and their revision in accordance with alternative conventions is straightforward.

This apparently not too well known method certainly deserves to be reviewed, and some of its features will be discussed in the next section, as part of the description of the present space-group algorithm; the (nowadays) rarely used dyadic formalism, in which Zachariasen's (1967) equations are expressed, is here replaced by the more familiar matrix and vector notation. The following section is devoted to a brief description of the geometrical characteristics of space-group symmetry operations and the corresponding symmetry elements, and the paper is concluded with examples of application of the above algorithms and some notes on the computer program in which they are implemented.

Algorithm for the generation of a space group

The basis of the present algorithm is Zachariasen's (1967) representation of the 32 crystallographic point groups in terms of cyclic groups and their products. The above representation can be briefly summarized by noting that (i) there are ten cyclic point groups

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(1, 2, 3, 4, 6, $\bar{1}$, m, $\bar{3}$, $\bar{4}$ and $\bar{6}$), (ii) fourteen point groups can be represented as products (see below) of cyclic point groups of the orders: 2, 3, 4 and 6, and point groups of order 2, and (iii) the remaining eight point groups involve products of three cyclic groups each or, more precisely, products of two groups of types (i) and (ii) above (*cf.* Table 2.5, Zachariasen, 1967).

Denoting a cyclic group by

$$\{H\} = \{H, H^2, \ldots, H^m = I\}, \qquad (1)$$

where m is the order of the group, I is its identity element and H is its generator (*e.g.* Ledermann, 1957), the above representation amounts to classifying the crystallographic point groups into the following three forms:

$$\text{(i) } \{Q\}, \text{ (ii) } \{Q\}\times\{R\} \text{ and (iii) } \{P\}\times[\{Q\}\times\{R\}], \qquad (2)$$

where P, Q and R are operators of proper or improper rotations that generate the corresponding cyclic point groups, and $\times$ denotes the operation of group multiplication, as defined below; either $\{Q\}$ or $\{R\}$ is a group of order 2.

The group products in (2), and in the rest of this paper, should be understood as follows.

(i) If $\{A\}$ and $\{B\}$ are groups, not necessarily cyclic, then their product, $\{C\} = \{A\}\times\{B\}$, is obtained as a set of *ordered* products of each element of $\{A\}$ by each element of $\{B\}$.

(ii) If the set $\{C\}$ is a product of the groups $\{A\}$ and $\{B\}$, then $\{C\}$ is a group *if and only if* $\{A\}$ and $\{B\}$ commute, *i.e.* if

$$\{C\} = \{A\}\times\{B\} = \{B\}\times\{A\} \qquad (3)$$

(Zachariasen, 1967, p. 248; Ledermann, 1957, p. 56).

(iii) It is not assumed that the individual elements of $\{A\}$ and $\{B\}$ also commute, *i.e.* that $A_iB_j = B_jA_i$ for any i and j; if this happens to be true, then $\{A\}\times\{B\}$ is a direct product of the two groups (*e.g.* Ledermann, 1957, p. 45).

The last restriction is missing from Zachariasen's definition of the direct product (Zachariasen, 1967, p. 248), and his reference to 'direct products', throughout the above representation, is therefore sometimes incorrect. In fact, only some of the point groups can be represented as direct products (in the generally accepted sense), but there is also little or no advantage in utilizing the nature of the group products in the present application. The points (i) and (ii) above are sufficient for the present purpose, and a group-theoretical classification of the products that occur in the generation of the point groups is outside the scope and beyond the requirements of this paper.

Table 1. *Product representation of crystallographic point groups*

The table lists the representations of the crystallographic point groups as products of cyclic groups (Zachariasen, 1967). Each cyclic group is generated by the operation, the symbol of which appears within the curly parentheses. The symbols are defined in Table 2. In order to obtain the matrix corresponding to a symbol with an overbar, *e.g.* $\bar{3}^c$, change the signs of all the matrix elements for this symbol, as given in Table 2. The product representations pertain to all the orientations of the axes which are needed for the generation of the 230 space groups. The second setting is used for the monoclinic system; to obtain the first setting, replace 2^b with 2^c.

Short symbol	Product representation	Short symbol	Product representation
1	$\{1\}$		$\{3^c\}\times\{\bar{2}^f\}^{(1),(5)}$
$\bar{1}$	$\{\bar{1}\}$	$3m$	$\{3^c\}\times\{\bar{2}^g\}^{(1),(6)}$
2	$\{2^b\}$		$\{3^q\}\times\{\bar{2}^e\}^{(2)}$
m	$\{\bar{2}^b\}$		
$2/m$	$\{\bar{1}\}\times\{2^b\}$		$\{\bar{3}^c\}\times\{2^f\}^{(1),(7)}$
222	$\{2^c\}\times\{2^a\}$	$\bar{3}m$	$\{\bar{3}^c\}\times\{2^g\}^{(1),(8)}$
$mm2$	$\{2^c\}\times\{\bar{2}^a\}$		$\{\bar{3}^q\}\times\{2^e\}^{(2)}$
mmm	$\{1\}\times[\{2^c\}\times\{2^a\}]$		
4	$\{4^c\}$	6	$\{6^c\}$
$\bar{4}$	$\{\bar{4}^c\}$	$\bar{6}$	$\{\bar{6}^c\}$
$4/m$	$\{\bar{1}\}\times\{4^c\}$	$6/m$	$\{\bar{1}\}\times\{6^c\}$
422	$\{4^c\}\times\{2^a\}$	622	$\{6^c\}\times\{2^f\}$
$4mm$	$\{4^c\}\times\{\bar{2}^a\}$	$6mm$	$\{6^c\}\times\{\bar{2}^f\}$
$\bar{4}2m$	$\{\bar{4}^c\}\times\{2^a\}$	$\bar{6}2m$	$\{\bar{6}^c\}\times\{2^f\}$
$\bar{4}m2$	$\{\bar{4}^c\}\times\{2^d\}$	$\bar{6}m2$	$\{\bar{6}^c\}\times\{2^g\}$
$4/mmm$	$\{\bar{1}\}\times[\{4^c\}\times\{2^a\}]$	$6/mmm$	$\{\bar{1}\}\times[\{6^c\}\times\{2^f\}]$
	$\{3^c\}^{(1)}$	23	$\{3^q\}\times[\{2^c\}\times\{2^a\}]$
3	$\{3^q\}^{(2)}$	$m\bar{3}$	$\{\bar{3}^q\}\times[\{2^c\}\times\{2^a\}]$
	$\{\bar{3}^c\}^{(1)}$	432	$\{3^q\}\times[\{4^c\}\times\{2^d\}]$
$\bar{3}$	$\{\bar{3}^q\}^{(2)}$	$\bar{4}3m$	$\{3^q\}\times[\{\bar{4}^c\}\times\{\bar{2}^d\}]$
		$m\bar{3}m$	$\{\bar{3}^q\}\times[\{4^c\}\times\{2^d\}]$
	$\{3^c\}\times\{2^f\}^{(1),(3)}$		
32	$\{3^c\}\times\{2^g\}^{(1),(4)}$		
	$\{3^q\}\times\{2^e\}^{(2)}$		

Notes: (1) hexagonal axes; (2) rhombohedral axes; (3) as in $P321$; (4) as in $P312$; (5) as in $P3m1$; (6) as in $P31m$; (7) as in $P\bar{3}m1$; (8) as in $P\bar{3}1m$.

Table 1 lists all the point groups, some of them in alternative representations, in terms of their cyclic-group building blocks, and Table 2 presents the twelve matrices of proper rotation which, taken together with inversion, suffice for the generation of the three-dimensional point groups (Zachariasen, 1967, p. 61) given in Table 1.

This representation of the point groups, which will be used as it stands in the generation of space groups, is particularly suitable for computation since the generating elements are explicit in the group symbols and the structure of the latter prescribes all the operations (here: matrix multiplication) to be performed; no iterative search for new elements, as implemented in other algorithms (Fokkema, 1975, 1983; Hall, 1981), is here required.

For example, the operations of the point group 32, in a representation suitable for the derivation of the

Table 2. *Point-group generators (proper rotations)*

The table defines the twelve rotation operators, which are needed in order to construct the product representations of the point groups, as given in Table 1.

$$1=\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}\quad 2^a=\begin{pmatrix}1&0&0\\0&\bar1&0\\0&0&\bar1\end{pmatrix}\quad 2^b=\begin{pmatrix}\bar1&0&0\\0&1&0\\0&0&\bar1\end{pmatrix}$$

$$2^c=\begin{pmatrix}\bar1&0&0\\0&\bar1&0\\0&0&1\end{pmatrix}\quad 2^d=\begin{pmatrix}0&1&0\\1&0&0\\0&0&\bar1\end{pmatrix}\quad 2^e=\begin{pmatrix}0&\bar1&0\\\bar1&0&0\\0&0&\bar1\end{pmatrix}$$

$$2^f=\begin{pmatrix}1&\bar1&0\\0&\bar1&0\\0&0&\bar1\end{pmatrix}\quad 2^g=\begin{pmatrix}1&0&0\\1&\bar1&0\\0&0&\bar1\end{pmatrix}\quad 3^q=\begin{pmatrix}0&0&1\\1&0&0\\0&1&0\end{pmatrix}$$

$$3^c=\begin{pmatrix}0&\bar1&0\\1&\bar1&0\\0&0&1\end{pmatrix}\quad 4^c=\begin{pmatrix}0&\bar1&0\\1&0&0\\0&0&1\end{pmatrix}\quad 6^c=\begin{pmatrix}1&\bar1&0\\1&0&0\\0&0&1\end{pmatrix}$$

Correspondence between the present and Zachariasen's symbols; l.h.s. present, r.h.s. Zachariasen (1967, Table 2.8):

$1=\mathbf{1}(a)$;	$2^a=\mathbf{2}'(o,t,c)$;	$2^b=\mathbf{2}(m)$;
$2^c=\mathbf{2}(o,t,c)$;	$2^d=\mathbf{2}''(o,t,c)$;	$2^e=\mathbf{2}'(hR)$;
$2^f=\mathbf{2}'(h)$;	$2^g=\mathbf{2}''(h)$;	$3^q=\mathbf{3}'(hR)$ and $\mathbf{3}'(c)$;
$3^c=\mathbf{3}(h)$;	$4^c=\mathbf{4}(t,c)$;	$6^c=\mathbf{6}(h)$;

where the letters *a*, *m*, *o*, *t*, *h* and *c* denote the triclinic, monoclinic, orthorhombic, tetragonal, hexagonal and cubic crystal families (Hahn & Vos, 1983), respectively, and the symbol *hR* indicates that the corresponding operation occurs in rhombohedral space groups.

space group $P321$, are obtained from Table 1 as

$$\{3^c\}\times\{2^f\}=\{1,3^c,(3^c)^2\}\times\{1,2^f\}$$
$$=\{1,3^c,(3^c)^2,2^f,3^c2^f,(3^c)^2 2^f\},\qquad(4)$$

followed by substitution of the appropriate matrices from Table 2 and evaluation of the matrix products. Note that (4) is not a direct product since, for example, 3^c2^f does not equal 2^f3^c. However, the same set of six matrices, in a different order, would be obtained upon evaluating the product $\{2^f\}\times\{3^c\}$ [*cf.* (3) above].

The coordinates of the general equivalent positions, for the space group $P321$, can now be obtained by premultiplying the vector (xyz), taken as a column vector, with the matrices in (4). Of course, all the symmorphic space groups can be derived in this manner, making use of Tables 1 and 2 and taking into account the appropriate Bravais lattices.

The above considerations are readily extended to the generation of non-symmorphic space groups. However, some relevant definitions and notation should first be recalled.

A space-group symmetry transformation is given by

$$\mathbf{r}'=P\mathbf{r}+\mathbf{t}+\mathbf{r}_L,\qquad(5)$$

where P is an operator of proper or improper rotation belonging to a point group, $\mathbf{r}_L$ is a lattice translation, $\mathbf{t}$ is a zero vector or a permissible translation not belonging to the lattice and the vectors $\mathbf{r}$ and $\mathbf{r}'$ denote the positions of two points with identical environments, *i.e.* equivalent positions. The space-group operator, involved in (5), is brought out by rewriting (5) in the Seitz (1935*b*) notation

$$\mathbf{r}'=(P|\mathbf{t}+\mathbf{r}_L)\mathbf{r}\qquad(6)$$

and the product of two space-group operators $(P|\mathbf{t})$ and $(Q|\mathbf{u})$ is

$$(P|\mathbf{t})(Q|\mathbf{u})=(PQ|P\mathbf{u}+\mathbf{t}),\qquad(7)$$

where the lattice vectors were taken as zero, as can be verified by making use of (5) and (6). The operator inverse to a space-group operator $(P|\mathbf{t})$ is given by

$$(P|\mathbf{t})^{-1}=(P^{-1}|-P^{-1}\mathbf{t})\qquad(8)$$

and the product of $(P|\mathbf{t})$ and $(P|\mathbf{t})^{-1}$ is seen to equal $(I|\mathbf{0})$, the identity element of the space group. The general form of a space-group operator, appearing in (6), can be rewritten as $(I|\mathbf{r}_L)(P|\mathbf{t})$, where $(I|\mathbf{r}_L)$ is an element of the translation subgroup of the space group. For further detailed explanations the reader is referred to the original paper by Seitz (1935*b*) or, more accessibly, to the explanatory sections of ITA83 (*e.g.* Wondratschek, 1983).

The following well-established results lead to the extension of the generation of the point groups to that of the space groups.

(i) The translation subgroup $\Gamma=\{(I|\mathbf{r}_L)\}$ is an invariant subgroup of the space group (Zachariasen, 1967; Ledermann, 1957).

(ii) Any space group, say G, can be represented by a factor group (*cf.* Ledermann, 1957, p. 102) which may consist of the following decomposition into cosets w.r.t. the invariant subgroup

$$\{(I|\mathbf{0})\Gamma,(P_2|\mathbf{t}_2)\Gamma,\ldots,(P_g|\mathbf{t}_g)\Gamma\}=G/\Gamma\qquad(9)$$

(Bertaut & Wondratschek, 1971, 1972; Wondratschek, 1983), where $(I|\mathbf{0})$ is the identity operation of the space group, $\mathbf{t}_i$ are zero vectors or space-group translations not belonging to Γ, P_i are point-group operators of proper or improper rotations and g is the order of the point group; g is also the order of the factor group, and the identity element of the latter is the invariant subgroup Γ.

(iii) The factor group G/Γ and the point group on which G/Γ is based are isomorphic (Ledermann, 1957; Wondratschek, 1983). Hence, there is a one-to-one correspondence between their generating elements.

It follows that a crystallographic factor group (omitting Γ) may have one of the following forms:

$$\text{(i) }\{(Q|\mathbf{u})\},\quad\text{(ii) }\{(Q|\mathbf{u})\}\times\{(R|\mathbf{v})\}$$
and
$$\text{(iii) }\{(P|\mathbf{t})\}\times[\{(Q|\mathbf{u})\}\times\{(R|\mathbf{v})\}],\qquad(10)$$

in correspondence with the point-group forms given by (2), where Q, R and P are point-group operators

and **u**, **v** and **t** are zero vectors or permissible space-group translations not belonging to Γ; the curled parentheses denote the set of all the different powers of the enclosed space-group operator (and generator). The corresponding forms of the full space groups follow by multiplying each of those in (10) with the appropriate translation subgroup Γ.

In order to generate a space group, we require the translation parts of the space-group generators, the rotation parts being given by Tables 1 and 2. This information is contained in the space-group data already available in all the main editions of *International Tables for X-ray Crystallography* (1935, 1952; ITA83), and is most easily accessible in the recent one, as will be shown in the last section.

For example, consider the point group 432 and the related space group $P4_132$. From Table 1 and (10), the factor group is given by

$$\{(3^q|\mathbf{t})\}\times[\{(4^c|\mathbf{u})\}\times\{(2^d|\mathbf{v})\}], \qquad (11)$$

where, in analogy with (1),

$$\{(3^q|\mathbf{t})\}=\{(3^q|\mathbf{t}),(3^q|\mathbf{t})^2,(3^q|\mathbf{t})^3\cong(I|\mathbf{0})\},$$
$$\{(4^c|\mathbf{u})\}=\{(4^c|\mathbf{u}),(4^c|\mathbf{u})^2,(4^c|\mathbf{u})^3,(4^c|\mathbf{u})^4\cong(I|\mathbf{0})\}$$

and

$$\{(2^d|\mathbf{v})\}=\{(2^d|\mathbf{v}),(2^d|\mathbf{v})^2\cong(I|\mathbf{0})\}; \qquad (12)$$

the sign $\cong$ indicates that the translational part of the product has been reduced to the reference unit cell, *i.e.* non-zero lattice vectors were subtracted. The components of the translations **t**, **u** and **v**, corresponding to the origin choice in *International Tables for X-ray Crystallography* (1952) and ITA83 for this group, are (0, 0, 0), $(\frac{1}{4},\frac{3}{4},\frac{1}{4})$ and $(\frac{3}{4},\frac{1}{4},\frac{1}{4})$, respectively. Making use of Table 2 and (7), the symbolic form of the factor group can now be readily expanded by computing all the products of the form $(3^q|\mathbf{t})^i(4^c|\mathbf{u})^j(2^d|\mathbf{v})^k$, where i, j and k are the exponents appearing in the expansion of the cyclic groups in (12).

A list of explicit space-group symbols, equivalent to the representations given in Tables 1 and 2, and in (10), is given by Zachariasen (1967), in correspondence with the 1935 edition of *International Tables for X-ray Crystallography*. These symbols, initially used in the present work, were modified to conform with the most recent source of space-group data (ITA83). A concise table, showing how to construct such symbols with the aid of ITA83, is given in the last section.

Zachariasen proposes three types of relations, which are necessary conditions for the validity of a set of space-group generators and represent restrictions on their translation parts (Zachariasen, 1967).

(i) Any generator (and, indeed, any space-group operator) must obey the relation

$$(Q|\mathbf{u})^m=(I|\mathbf{r}_L), \qquad (13)$$

where m is the order of Q, $\mathbf{r}_L$ is a lattice vector and I is the unit matrix. Equation (13) is of fundamental importance in the actual generation and description of space-group operations.

(ii) If the factor group is of the form

$$G/\Gamma=\{(Q|\mathbf{u})\}\times\{(R|\mathbf{v})\}, \qquad (14)$$

where one of the generators is of order 2, we must have

$$(Q|\mathbf{u}+\mathbf{r}_L)=(R|\mathbf{v})(Q|\mathbf{u})(R|\mathbf{v}), \qquad (15)$$

where $\mathbf{r}_L$ is a lattice vector. The generators $(Q|\mathbf{u})$ and $(R|\mathbf{v})$ above must correspond to the first and second point-group generators in the relevant entries of Table 1, respectively. Relation (15) is also used by Zachariasen (1967) in examples of derivations of the possible space groups that are based on a given point group.

(iii) If the factor group is of the form

$$G/\Gamma=\{(P|\mathbf{t})\}\times[\{(Q|\mathbf{u})\}\times\{(R|\mathbf{v})\}], \qquad (16)$$

the generators $(Q|\mathbf{u})$ and $(R|\mathbf{v})$ must obey relation (15), and the following equation has to be satisfied

$$(Q|\mathbf{u}+\mathbf{r}_L)=(P|\mathbf{t})^{-1}(Q|\mathbf{u})^j(R|\mathbf{v})^k(P|\mathbf{t})^l, \qquad (17)$$

where j, k and l are integers, uniquely associated with a point group [*cf.* equation [2.115*b*], Zachariasen, 1967]. As in (15) above, the order of the generators must follow Table 1.

The integer triplets jkl in (17) were found to assume the following values: 121 (for *mmm*, 4/*mmm* and 6/*mmm*), 211 (for 23 and $m\bar{3}$), 322 (for 432 and $\bar{4}3m$) and 325 (for $m\bar{3}m$).

Equations (13)–(17) have been used in testing computer-adapted symbols for all the space groups. An expanded form of (13) is most useful in the decomposition of the translation part of a space-group operation into its intrinsic (screw axis or glide plane) and location-dependent components (Wondratschek & Neubüser, 1967; Fischer & Koch, 1983).

The coordinates of the general equivalent positions, computed by the present method, reproduce those given in ITA83 for space groups with *P*-type Bravais lattices, and sometimes differ from those given in the above reference by centering translations of non-*P* lattices. It appears difficult to achieve a complete consistency, regarding this formal matter, however. It was found advisable to omit the reduction of the translation parts of the space group operations modulo lattice vectors with fractional components, at least until some definite rules for such reduction are established.

The present algorithm is readily adapted to non-standard settings. If, for example, the position vector of a point is transformed from the old (crystal) axes and origin to new ones by

$$\mathbf{r}_{(\text{new})}=T\mathbf{r}_{(\text{old})}+\boldsymbol{\rho}, \qquad (18)$$

the corresponding relation between the space-group

generators is

$$(P|\mathbf{t})_{\text{new}} = (T|\boldsymbol{\rho})(P|\mathbf{t})_{\text{old}}(T|\boldsymbol{\rho})^{-1}, \qquad (19)$$

where T is a transformation matrix and $\boldsymbol{\rho}$ is the origin-shift vector (see *e.g.* Arnold, 1983). Similar transformations can be easily devised if it is desired to utilize crystallographic space-group operations in computations referred to a Cartesian system. In any case only the generators have to be transformed, whereafter their expansion into the required set of space-group operators follows as outlined in the above example.

It may also be of interest to compare the space-group generators chosen in this study with those used for *International Tables for Crystallography* (1983). As pointed out above, the present choice is dictated by the cyclic-group representation (Table 1) which ensures the ease of the construction of a well-defined and efficient algorithm. In ITA83, the choice of the generators and generating procedures was such as to ensure a 'transparent' ordering of the coordinates of the equivalent positions and an easy recognition of important subgroups (Wondratschek, 1983). It appears that the purpose has been achieved in both cases.

Since in the present algorithm all the space groups which are based on a given point group are generated in the same way [*cf.* Table 1, (10) and last section], and the same procedure was followed in the generation of the space-group tables in ITA83, there is a one-to-one correspondence between the ordering of the positions in both cases. The preferable ordering, as given in ITA83, is thus achieved with the aid of a simple sorting procedure, as would be the case for any ordering scheme involving a point-group-like arrangement.

The space-group tables in ITA83 require up to five generators for a space group, while in the present case only up to three generators are needed (both numbers do not include lattice translations). A smaller set of generators becomes advantageous when the space-group symbol, whether computer-adapted or not, is to contain all of them explicitly. This is the case in the present study, since the computer-adapted space-group symbol (see last section) serves here as the only input item required for the generation of a space group.

Orientation and location of symmetry elements

The matrix-vector representation of a space-group operator, secured as described above, contains all the information that is required for a complete geometrical characterization of the space-group operation and the corresponding symmetry element. Procedures for doing this are well documented in the literature and two detailed articles devoted to this subject have been published (Wondratschek & Neubüser, 1967; Fischer & Koch, 1983). Algorithms for the determination of (i) the type of the rotation (proper or improper), (ii) the angle of the rotation, (iii) the order of the rotation part (as an element of the point group), and (iv) the decomposition of the translation part of the space-group operation into its intrinsic and location-dependent components, are given in the above references, and detailed examples are contained in the second one (Fischer & Koch, 1983). We shall comment below on an alternative method for the determination of the orientation of axes of rotation, and will deal with the location vectors of the symmetry elements in somewhat greater detail.

Orientation of the axis of rotation

A lattice vector parallel to an axis of rotation can be obtained by solving the eigenvalue equations: $P\mathbf{r} = \mathbf{r}$ or $P\mathbf{r} = -\mathbf{r}$, according as P corresponds to a proper or an improper rotation, respectively (*e.g.* Wondratschek & Neubüser, 1967), and suitably normalizing the components of the appropriate eigenvector $\mathbf{r}$. The following approach is often a useful alternative to the above.

Given a space-group operation, say $(P|\mathbf{t})$, consider the matrices

$$[P]_1 = I + P + P^2 + \ldots + P^{m-1} \qquad (20)$$

and

$$[P]_2 = I - P + P^2 + \ldots + (-1)^{m-1}P^{m-1}, \qquad (21)$$

where $m = 2$, 3, 4 or 6 is the order of P (*i.e.* $P^m = I$), and let $\mathbf{r}_S$ be a lattice vector which is neither perpendicular nor parallel to the axis of rotation. Decomposing $\mathbf{r}_S$ into its components along and normal to the axis, it is easily shown that a lattice vector parallel to the axis of rotation can be directly obtained as

$$\mathbf{r}_P = \begin{cases} [P]_1\mathbf{r}_S, & \text{if } P \text{ is a proper rotation} \\ [P]_2\mathbf{r}_S, & \text{if } P \text{ is an improper rotation.} \end{cases} \qquad (22)$$

The vector $\mathbf{r}_S = (1, 3, 5)$ can serve the above purpose for all the symmetry operations in the standard (ITA83) space-group settings.

The components of the vectors $\mathbf{r}_P$, $\mathbf{r}_S$ and $P\mathbf{r}_S$ can now be used, as described by Fischer & Koch (1983), in the determination of the sense of the rotation (where appropriate), and the matrix $[P]_1$ is needed anyway for the decomposition of the translation part of the space-group operation into its intrinsic and location-dependent components (*e.g.* Wondratschek & Neubüser, 1967; Fischer & Koch, 1983). The matrix $[P]_1$ is equivalent to Zachariasen's (1967) 'characteristic dyadic', frequently used in his study.

Location of symmetry elements

In order to specify the location of a symmetry element (axis or plane), we require its orientation and the

coordinates of any point located on the element under consideration. A general location vector is given by the sum of a vector with variable components [based on $\mathbf{r}_p$ in (22)] and the position vector, say $\mathbf{x}$, of the above fixed point. As pointed out in nearly all the references that deal with the geometry of space-group symmetry elements, the vector $\mathbf{x}$ must satisfy the equation

$$P\mathbf{x}+\mathbf{t}_{\rm loc}=\mathbf{x} \quad \text{or} \quad (I-P)\mathbf{x}=\mathbf{t}_{\rm loc}, \tag{23}$$

where I is the unit matrix and $\mathbf{t}_{\rm loc}$ is the location-dependent component of the space-group operation $(P|\mathbf{t})$. Of course, the intrinsic part of the translation $\mathbf{t}$ is not relevant, and if $\mathbf{t}_{\rm loc}=0$ the element passes through (or is located on) the origin. However, a systematic computation of such location vectors still deserves some comments.

If P corresponds to an axis of inversion other than $\bar{2}=m$, the solution is obvious since, in this case, there must be one and only one point (a special position) satisfying (23), and the matrix $(I-P)$ is then not singular.

For P representing a twofold axis of proper rotation or a plane of reflection, the translation component $\mathbf{t}_{\rm loc}$ is perpendicular to the element and, in either case, the solution of (23) can be written as $\mathbf{x}=\mathbf{t}_{\rm loc}/2+\mathbf{x}_p$, where $\mathbf{x}_p$ is the indeterminate part of $\mathbf{x}$ and can be set equal to a zero vector. In general, for $P=2$, $\mathbf{x}_p$ is parallel to the twofold axis and for $\mathbf{P}=m$, $\mathbf{x}_p$ is parallel to the reflection plane.

The remaining elements are threefold, fourfold and sixfold axes of proper rotation, the component of $\mathbf{x}$ parallel to an axis being indeterminate. In standard representations of the space groups (*e.g.* ITA83), any of these axes is either parallel to one of the basis vectors or to one of the body diagonals of the unit cell. If, for example, an axis is parallel to **a**, the first (x) component of the vector $\mathbf{x}$ is indeterminate and the remaining two components are solved for by deleting the first row and first column of the matrix $(I-P)$ in (23). Axes parallel to **b** and **c** are treated analogously.

The case of an axis being parallel to a body diagonal is less obvious, since the singularity of the matrix $(I-P)$ cannot be dealt with as simply as for the [100], [010] and [001] orientations above. The same problem may arise for any axis of proper rotation ($n>2$), which is oriented in a general direction. The solution is (i) to transform (23) to a system such that one of its basis vectors coincides with the vector parallel to the axis of rotation, (ii) solve (23) for the determinable components of $\mathbf{x}$, while equating the indeterminate one to zero, and (iii) transform the solution vector back to the original system. In standard space-group settings, the above concerns only the threefold axes in the cubic system, for which $\mathbf{t}_{\rm loc}$ is not a zero vector.

The general forms of the location vectors of the various symmetry elements can now be obtained from their 'axis eigenvectors' $\mathbf{r}_P$ [*cf.* (22)] and the coordinates of the points through which the elements are passing. If, for example, a threefold axis in a cubic space group is parallel to $[1\bar{1}\bar{1}]$ and is found to pass through the point $(\frac{1}{6}, -\frac{1}{6}, \frac{1}{3})$, a general location vector for this axis can be written as $(x+\frac{1}{6}, \bar{x}-\frac{1}{6}, \bar{x}+\frac{1}{3})$. Of course, any vector with components $(\delta, -\delta, -\delta)$ can now be added to the general location vector, without changing its geometrical significance. Other rotation and inversion axes are treated in the same manner.

For mirror or glide-plane operations, the plane normal is rotated through 90° about a line contained in the plane, the components of the rotated lattice vector are replaced by the appropriate variables and the fixed vector $\mathbf{x}$ is added. For example, consider a mirror plane in a hexagonal space group, with plane normal [100] and passing through the origin. After rotating the normal through 90° about the z axis, its direction coincides with that of [120] (an in-plane lattice vector) and the location vector for this symmetry element can be written as $(x, 2x, z)$. This is, of course, a special position.

Results and programming considerations

The algorithms described in the above two sections were implemented in a computer program, which was written in Fortran and has been run on the CDC 6600 and Cyber computers at the Tel-Aviv University Computation Center. The results obtained are illustrated by the development and characterization of the cubic space group $Pa\bar{3}$ (No. 205) in Table 3.

The symmetry operations are sorted according to the ordering scheme of ITA83 (different ordering schemes are used in other versions of the program). The column with the heading T(PROP) lists the screw-axis and glide-plane translations, where present, and the vectors T(DISP) contain the location-dependent components of the space-group operations (*cf.* $\mathbf{t}_{\rm loc}$ above). The last column presents the location vectors in their general forms, derived as described at the end of the previous section. These vectors differ from those given in ITA83 by vectors proportional to the axis eigenvectors (see above). It is immediately seen which vectors correspond to special positions, and the orientations of the axes and planes can be read off the variable parts of the location vectors. It may be noted that the complete location vectors for 3BAR ($=\bar{3}$) operations furnish a geometrical description of the corresponding axes, while only the fixed parts of these vectors are coordinates of special positions.

The input, from which the space-group information shown in Table 3 has been generated, consists of the following symbol:

PCC$I3Q000$P2C606$P2A660. (24)

In this computation a point-group code was also used

Table 3. *Derivation and characterization of the space group Pa$\bar{3}$*

The output listing of program *SPGRGEN*, given in the table shows the elements (order of axis, sense of rotation and type), coordinates of the general equivalent positions, screw-axis and glide-plane translations [T(PROP)], location-dependent components of the translations [T(DISP)], and possible forms of general location vectors of the symmetry elements for this space group. Explanations are given in the text.

SPACE GROUP - PA3BAR NO.205 ;ITS GENERATORS ARE;

(I3Q; 0, 0, 0) (P2C;1/2, 0,1/2) (P2A;1/2,1/2, 0)

CUBIC LATTICE TYPE - P CENTROSYMMETRIC

24 OPERATIONS GENERATED. CLOSURE AND INVERSE TESTS O.K.

	ELEMENT	EQUIVALENT POSITIONS	T(PROP)	T(DISP)	LOCATION VECTOR
1	1	+ X + Y + Z	(0, 0, 0)	(0, 0, 0)	(0 , 0 , 0)
2	2	1/2 - X - Y 1/2 + Z	(0, 0, 1/2)	(1/2, 0, 0)	(1/4 , 0 , +Z)
3	2	- X 1/2 + Y 1/2 - Z	(0, 1/2, 0)	(0, 0, 1/2)	(0 , +Y, 1/4)
4	2	1/2 + X 1/2 - Y - Z	(1/2, 0, 0)	(0, 1/2, 0)	(+X, 1/4 , 0)
5	3(+)	+ Z + X + Y	(0, 0, 0)	(0, 0, 0)	(+X, +X, +X)
6	3(+)	1/2 + Z 1/2 - X - Y	(0, 0, 0)	(1/2, 1/2, 0)	(1/3 -X, 1/6 +X, -1/6 -X)
7	3(+)	1/2 - Z - X 1/2 + Y	(0, 0, 0)	(1/2, 0, 1/2)	(1/6 +X, -1/6 -X, 1/3 -X)
8	3(+)	- Z 1/2 + X 1/2 - Y	(0, 0, 0)	(0, 1/2, 1/2)	(-1/6 -X, 1/3 -X, 1/6 +X)
9	3(-)	+ Y + Z + X	(0, 0, 0)	(0, 0, 0)	(+X, +X, +X)
10	3(-)	- Y 1/2 + Z 1/2 - X	(-1/3, 1/3, 1/3)	(1/3, 1/6, 1/6)	(1/6 +X, 1/6 -X, -X)
11	3(-)	1/2 + Y 1/2 - Z - X	(1/3, 1/3, -1/3)	(1/6, 1/6, 1/3)	(1/6 -X, -X, 1/6 +X)
12	3(-)	1/2 - Y - Z 1/2 + X	(1/3, -1/3, 1/3)	(1/6, 1/3, 1/6)	(-X, 1/6 +X, 1/6 -X)
13	1BAR	- X - Y - Z	(0, 0, 0)	(0, 0, 0)	(0 , 0 , 0)
14	2BAR	1/2 + X + Y 1/2 - Z	(1/2, 0, 0)	(0, 0, 1/2)	(+X, +Y, 1/4)
15	2BAR	+ X 1/2 - Y 1/2 + Z	(0, 0, 1/2)	(0, 1/2, 0)	(+X, 1/4 , +Z)
16	2BAR	1/2 - X 1/2 + Y + Z	(0, 1/2, 0)	(1/2, 0, 0)	(1/4 , +Y, +Z)
17	3(+)BAR	- Z - X - Y	(0, 0, 0)	(0, 0, 0)	(+X, +X, +X)
18	3(+)BAR	1/2 - Z 1/2 + X + Y	(0, 0, 0)	(1/2, 1/2, 0)	(-X, 1/2 +X, 1/2 -X)
19	3(+)BAR	1/2 + Z + X 1/2 - Y	(0, 0, 0)	(1/2, 0, 1/2)	(1/2 +X, 1/2 -X, -X)
20	3(+)BAR	+ Z 1/2 - X 1/2 + Y	(0, 0, 0)	(0, 1/2, 1/2)	(1/2 -X, -X, 1/2 +X)
21	3(-)BAR	- Y - Z - X	(0, 0, 0)	(0, 0, 0)	(+X, +X, +X)
22	3(-)BAR	+ Y 1/2 - Z 1/2 + X	(0, 0, 0)	(0, 1/2, 1/2)	(+X, -X, 1/2 -X)
23	3(-)BAR	1/2 - Y 1/2 + Z + X	(0, 0, 0)	(1/2, 1/2, 0)	(-X, 1/2 -X, +X)
24	3(-)BAR	1/2 + Y + Z 1/2 - X	(0, 0, 0)	(1/2, 0, 1/2)	(1/2 -X, +X, -X)

for sorting the operations, and the space-group identifier (PA3) and number were appended to the symbol (24), in the same card image, for output only.

The first three characters in (24) denote the lattice type, crystal system and status of centrosymmetry. Each generator occupies a six-character field, following a separator ($), in which the first character is I or P according as the rotation is proper or improper, respectively, the second and third characters contain the code of the rotation matrix (as in Table 2, with superscripts converted to upper-case letters) and the last three characters give the components of the space-group translation, in units of $\frac{1}{12}$. If sorting and/or a test of the generators [with (13), (15) and (17) above] are needed, point-group codes and/or the *jkl* triplets [see (17)] are appended to the symbol.

The symbol in (24) is most easily decoded, and only a minimum number of conventions need be incorporated into the program, which thus readily admits alternative choices of the origin and modified space-group settings. The necessary conventions amount to Table 2 and translation vectors associated with lattice-type letters. A separate file with such symbols seems to be preferable to a list included in, say, a DATA block of the program since it can be independently tested for relations between the generators, after any modifications or additions have been introduced.

With regard to computing time, only a small fraction of it is spent on developing the space group from its symbol, the slowest item being comprehensive tests for closure and the presence of an inverse element to each given one. In particular, the inverse test was found to be rather sensitive. However, these tests can often be relaxed, *e.g.* when the space-group symbols have previously been examined for internal consistency. A derivation of the 230 space groups, in all their representations given in ITA83, with the aid of the slowest version of the program (tests for closure and inverse, and description of the symmetry operations included), required about 37 s computing time on a Cyber 170-855. The program thus appears to be a suitable tool for computerized 'space-group look up', whether for an inspection of the results, or their transfer to subsequent calculations in numeric or symbolic format.

The above computations were initially carried out with space-group symbols which were made compatible with Vol. I of *International Tables for X-ray Crystallography* (1952). While this paper was being written, the author has been given the opportunity to compare the old conventions with those on which the new *International Tables for Crystallography* (ITA83) are based. It was therefore possible to establish a link between the input to the present program and the new source of space-group data. The comparison was

Table 4. *A concise reference to the generators of all the 230 crystallographic space groups*

The first column of the table lists the short symbols of the 32 crystallographic point groups, in all the relevant orientations. The second-column entry, corresponding to a given point group, contains the serial numbers of the general equivalent positions (ITA83), which completely specify the generators of all the space groups based on this point group. For further explanations and example, see text and table footnotes.

Short symbol	Generator(s)
Triclinic	
1	(1)
$\bar{1}$	(2)
Monoclinic	
2	(2)
m	(2)
2/*m*	(3), (2)
Orthorhombic	
222	(2), (4)
*mm*2	(2), (4)
mmm	(5), (2), (4)
Tetragonal	
4	(3)
$\bar{4}$	(3)
4/*m*	(5), (3)
422	(3), (5)
4*mm*	(3), (6)
$\bar{4}$2*m*	(3), (6)
$\bar{4}$*m*2	(3), (7)
4/*mmm*	(9), (3), (6)
Trigonal*	
3 (*hP*)	(2)
3 (*hR*, *hRh*)	(2)
$\bar{3}$ (*hP*)	(5)
$\bar{3}$ (*hR*, *hRh*)	(5)
312 (*hP*)	(2), (6)
321 (*hP*)	(2), (5)
32 (*hRr*)	(2), (4)
32 (*hRh*)	(2), (5)
3*m*(*hP*)	(2), (6)
3*m*1(*hP*)	(2), (5)
3*m* (*hRr*)	(2), (4)
3*m* (*hRh*)	(2), (5)
$\bar{3}$1*m*(*hP*)	(8), (6)
$\bar{3}$*m*1(*hP*)	(8), (5)
$\bar{3}$*m* (*hRr*)	(8), (4)
$\bar{3}$*m* (*hRh*)	(8), (5)
Hexagonal	
6	(6)
$\bar{6}$	(6)
6/*m*	(7), (6)
622	(6), (8)
6*mm*	(6), (8)
$\bar{6}$2*m*	(6), (8)
$\bar{6}$*m*2	(6), (12)
6/*mmm*	(13), (6), (8)
Cubic	
23	(5), (2), (4)
m$\bar{3}$	(17), (2), (4)
432	(5), (16), (13)
$\bar{4}$3*m*	(5), (15), (14),
m$\bar{3}$*m*	(29), (16), (13)

* Remarks on the trigonal space groups.

(*a*) The symbols '*hP*' and '*hR*' denote the hexagonal and rhombohedral Bravais lattices, respectively.

(*b*) The symbols '*hRr*' and '*hRh*', following the short point-group symbol, indicate that the generators listed correspond to the ITA83 representation of the relevant space groups in rhombohedral and hexagonal axes, respectively.

(*c*) Conventional point-group symbols are sometimes modified to suggest the orientations of the pertinent space groups. For example, point group 32, when given as 312, indicates that it leads to the space group *P*312 *etc.*

greatly facilitated by the facts that (i) ITA83 lists the space-group operations, based on a given point group, in the same order of their rotation parts (see above), and (ii) the equivalent positions and the corresponding symmetry operations, in ITA83, are numbered. Hence, the generators defined by Tables 1 and 2 and by (10) can now be represented as serial numbers of the general equivalent positions appearing in the above reference. Such a definition of the 230 crystallographic space groups, in the context of the present algorithm, is provided by Table 4 which lists the point groups and the serial numbers of the general equivalent positions (in ITA83) that correspond to the generators in Table 1.

For example, let us construct the space-group symbols [*cf.* (24)] for the space groups $Pm\bar{3}n$ (No. 223) and $Pn\bar{3}m$ (No. 224, origin at centre). These space groups are based on the point group $m\bar{3}m$, and the serial numbers of the generators, (29), (16) and (13) in Table 4, correspond to $(\bar{z}, \bar{x}, \bar{y})$, $(\bar{y}+1/2, x+1/2, z+1/2)$ and $(y+1/2, x+1/2, \bar{z}+1/2)$ for $Pm\bar{3}n$ and to $(\bar{z}, \bar{x}, \bar{y})$, $(\bar{y}, x+1/2, z+1/2)$ and $(y+1/2, x+1/2, \bar{z})$ for $Pn\bar{3}m$, respectively. The required symbols are readily constructed, using Tables 1 and 2 and considering the structure of the space-group symbol described above [*cf.* (24)].

We thus obtain

PCC$I3Q000$P4C666$P2D666 for $Pm\bar{3}n$ (25)

and

PCC$I3Q000$P4C066$P2D660 for $Pn\bar{3}m$. (26)

The origins of these two space groups are the same in the new and old editions of *International Tables for X-ray Crystallography*. However, the use of the new source of space-group data is much easier, owing to the consistent point-group like arrangement.

Table 4 leads to all the representations of the space groups that are given in ITA83.

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Geometric Units in Hexagonal and Rhombohedral Space Groups

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Abstract

Hexagonal space groups, *i.e.* those with an *hP* lattice, are classified from the geometric-unit viewpoint by considering hexagonal crystal structures as combinations and permutations of some basic hexagonal prisms. Geometric units are the Dirichlet domains of the Wyckoff positions with the highest point-group symmetry in the space group. In this classification, there are six types of hexagonal space groups. Type *h*1 consists of two independent geometric units of the same symmetry per crystallographic cell; in type *h*2, the two units are identical, but differently oriented. Type *h*3 has six independent geometric units, again of the same point-group symmetry, but the six units can be made up of three pairs, each consisting of two identical units, thus giving rise to type *h*4. There are subclasses in types *h*1 and *h*3. Centers of geometric units in *h*1(*a*) and *h*3(*a*) are uniquely defined by intersections of point-group symmetry elements, whereas those in *h*1(*b*) and *h*3(*b*) are not because the space groups in these subtypes are hemimorphic. Therefore, the two units along the polar axis may be combined as one. Type *h*5 consists of three units, each turned 120° from its neighbors owing to the screw axis 3_1, 3_2, 6_2 and 6_4. Similarly, type *h*6 has six units due to screw axes 6_1 and 6_5, and adjacent units are 60° apart. Rhombohedral space groups show two types of patterns: type *r*1 has two independent, and type *r*2 two identical, units. The h.c.p. and related structures are used to demonstrate the application of geometric units to crystal-structure descriptions.

Introduction

A recurring problem in finding a model for the solution of a crystal structure and its interpretation is to identify some convenient units that, by easy symmetry operations, will enable the construction of the entire structure. In this respect, asymmetric units, topological units (Wells, 1977), crystal chemical units, symmetry-related units (Kennard, Speakman & Donnay, 1967), building units (Lima-de-Faria & Figueiredo, 1976) and crystallographic cells have been used. For cubic crystal structures, Chieh (1979) suggested geometric units based on the construction of polyhedra, a proposal which differs from the previous ones in that it deals mainly with the symmetrical distribution of the atoms in the structure, rather than their connectivity or framework. The classification and description of cubic space groups in terms of geometric units were later given by Chieh, Burzlaff & Zimmermann (1982). The concept of geometric units was extended to tetragonal space groups by Chieh (1983), and some advantages were pointed out.

Applications of geometric units to cubic crystal structures have been given in previous publications (Chieh, 1980, 1982, 1983). Their application to the solution of a crystal structure and its subsequent interpretation was exemplified by the paper on anhydrous zinc bromide (Chieh & White, 1984). The present paper deals with the hexagonal and rhombohedral space groups.

Early work on the classification of cubic space groups by geometric units was somewhat intuitive. As more work on the theoretical aspects of space groups developed (see Gubler, 1982; Fischer & Koch, 1983; Burzlaff & Zimmermann, 1980) it became apparent that the classification follows the results of Euclidean normalizers of space groups. The purpose of geometric units is to divide a crystal structure into polyhedral units that have the same shape, volume and point-group symmetry.

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