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Derivation of the Normalizers of the Space Groups

By M. B. Boisen Jr

Department of Mathematics, Virginia Polytechnic Institute and State University, Blacksburg, VA 24061, *USA*

G. V. Gibbs

Department of Geological Sciences, Virginia Polytechnic Institute and State University, Blacksburg, VA 24061, *USA*

and H. Wondratschek

Institut für Kristallographie der Universität (TH), Kaiserstrasse 12, *D*-7500 *Karlsruhe, Federal Republic of Germany*

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Abstract

A method for the derivation of the affine normalizers of the space groups using matrix methods is presented. Published lists of normalizers have been verified, using matrix methods, both by hand and by computer. Generating matrices for the affine normalizers of triclinic and monoclinic space groups are listed.

1. Listings of normalizers in the literature

Because of the recent interest in normalizers of space groups, it is important that accurate lists of these normalizers be available in the literature. For the definition of normalizers, see any standard text on group theory or *International Tables for Crystallography* (1987), Vol. A (*IT*), §§ 8.3.6 or 15.2.

Normalizers of space groups were used in crystallography long before crystallographers were aware of the formal definition of a normalizer and its properties. The earliest list of normalizers of crystallographic groups we could find is that in Seitz (1935*a*) which presents, on p. 311, the orthogonal normalizers of the holohedries of space lattices. Normalizers of the crystallographic point groups have been published by Galiulin, Nardov, Shustov & Delone (1976) and Galiulin (1978). Tables of structure invariants and semi-invariants used in the solution of a crystal structure by direct methods (Hauptman & Karle, 1953, 1956, 1959; Karle & Hauptman, 1961) involve normalizers: in their tables, for each space group, $\mathfrak{G}$, the equivalence class of 'permissible origins' that contains 0,0,0 is generated by the translations that appear as 'additional generators of $\mathfrak{N}_{\mathfrak{E}}(\mathfrak{G})$ and $\mathfrak{N}_{\mathfrak{A}}(\mathfrak{G})$' in Table 15.3.2 of *IT* (1987). Similarly, tables appearing in Volume IV of *International Tables for X-ray Crystallography* (1974) and Giacovazzo (1980) are based on these translations.

To our knowledge, the first listings of normalizers of plane groups and three-dimensional space groups were published in 1968. For plane groups, Fischer (1968, Table 1) listed 'automorphism groups' of those 13 plane-group types whose normalizers have only discrete translations and are isomorphic to plane groups. These automorphism groups are isomorphic to their corresponding Euclidean normalizers because the centralizer of each of these plane groups is trivial. In the three-dimensional case, Hirshfeld (1968, Table 2) listed the 'Cheshire groups' for all 230 space-group types. Burzlaff & Zimmermann (1980) have since recognized that these are the Euclidean normalizers of the space groups. Dzyabchenko (1983) has extended Hirshfeld's approach and has listed the affine normalizers of the monoclinic and orthorhombic space groups.

In 1975, Koch & Fischer derived the automorphism group of each space group, with the exception of the triclinic and monoclinic ones, by determining the group of affine mappings that map the framework of symmetry elements of the space group onto itself. A list of the affine normalizers, automorphism groups and centralizers is given by Burzlaff & Zimmermann (1980, Table 3) and by Billiet, Burzlaff & Zimmermann (1982). These authors also clarified some of the confusion that existed in the literature by carefully stating the mathematical relationships between the normalizer, the centralizer and the automorphism group of a space group. Fischer & Koch (1983) have since given a comprehensive overview of the history of the applications of normalizers of space groups and have published tables of the Euclidean normalizers which are much more detailed than those published by Hirshfeld (1968). More recently, Dzyabchenko (1983, 1986) has applied affine normalizers to find optimal packings of molecular crystals.

Remarks on the derivation of normalizers of space groups usually invoke diagrams of symmetry elements as visual aids by the use of such phrases as 'the symmetry of the framework of symmetry elements'

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or the 'symmetry of the symmetry diagrams' (Hauptman & Karle, 1953, pp. 11, 12; 1956, p. 47; 1959, p. 95; Fischer, 1968; Hirshfeld, 1968; Fischer, 1971; Koch & Fischer, 1975; Fischer & Koch, 1983). Burzlaff & Zimmermann (1980) derived their list of normalizers from Koch & Fischer's (1975) list of automorphism groups. Parthé & Gelato (1984) listed Hirschfeld's (1968) data in their paper on the standardization of inorganic crystal structures. Consequently, it appears that in these papers the normalizers were found by determining the symmetry of the framework of symmetry elements shown in the space-group diagrams displayed in the various editions of *International Tables* (*Internationale Tabellen zur Bestimmung von Kristallstrukturen*, 1935; *International Tables for X-ray Crystallography*, 1952; *International Tables for Crystallography*, 1983) or similar publications. Since the affine normalizers of the triclinic and monoclinic space groups cannot be obtained in this way, they were not included in the early lists.

Using Sayari & Billiet's (1977) data, Billiet, Burzlaff & Zimmermann (1982) constructed a list of the affine normalizers of the triclinic and monoclinic space groups. Following Gubler (1982*b*), a list of the affine normalizers of the plane groups can be derived from Tables 1 to 3 of Sayari, Billiet & Zarrouk (1978) by replacing the condition $\det(M) \geq 1$ with $\det(M) = \pm 1$. Gubler (1982*b*, p. 6) suggested, without giving a proof, that the normalizers could be found by inspecting the framework of symmetry elements. However, he was careful to caution that such a strategy 'needs the support of an exact mathematical method'. In presenting his strategy, Gubler (1982*a*, *b*) observed that two steps of the procedure 'require some intuition, and insofar the general problem is not solved'. As for several others of those mentioned above, Gubler's list of normalizers is not error free.

Finally, in 1987, *IT* was supplemented in a second edition by the inclusion of § 15 which contains a list of the Euclidean and affine normalizers for the plane and space groups. In these lists for all plane groups $\mathfrak{G}$ (except the oblique ones) and all space groups $\mathfrak{G}$ (except the triclinic and monoclinic ones) each normalizer $\mathfrak{N}(\mathfrak{G})$ is characterized by its symbol and a primitive basis for the lattice part of its translation subgroup. Furthermore, additional generators, for both the Euclidean $\mathfrak{N}_{\mathfrak{E}}(\mathfrak{G})$ and the affine $\mathfrak{N}_{\mathfrak{A}}(\mathfrak{G})$ normalizers of $\mathfrak{G}$, as well as the indices of $\mathfrak{G}$ in $\mathfrak{N}_{\mathfrak{E}}(\mathfrak{G})$ and $\mathfrak{N}_{\mathfrak{A}}(\mathfrak{G})$ are listed. The normalizers of the oblique plane groups and the triclinic and monoclinic space groups are listed by the general entries of their matrix-column pairs. No errors in the list of § 15 have been found so far.

In this paper we present an algebraic procedure by which the affine normalizers of the space groups can be obtained. We applied this procedure to plane and three-dimensional space groups. In principle, the procedure does not depend on the dimension of space. There may be, however, technical difficulties for higher dimensions. For four dimensions, listing the affine space-group normalizers should not be too difficult because lists of the space groups and of the corresponding point-group normalizers have been provided by Brown, Bülow, Neubüser, Wondratschek & Zassenhaus (1978).

2. The calculation of the normalizers of the space groups

The following discussion assumes that a real n-dimensional point space is given together with a coordinate system consisting of a basis and an origin. For a discussion of the definition and properties of n-dimensional point spaces, affine spaces and mappings see Greub (1975). Each point in point space can be represented by an $n\times 1$ column of its coordinates. An affine mapping defined on this space maps each point X to a point X' such that

$$x' = \mathbf{A}x + \mathbf{a}$$

where x and x' are the columns representing X and X', respectively, and where $\mathbf{A}$ is a real $n\times n$ matrix and $\mathbf{a}$ is a real $n\times 1$ column. In order to emphasize that this is a single mapping, the symbol $(\mathbf{A}, \mathbf{a})$ is used and the equation is written as

$$x' = (\mathbf{A}, \mathbf{a})x.$$

Instead of $(\mathbf{A}, \mathbf{a})$, the symbol $(\mathbf{A}|\mathbf{a})$ is also used and is called the Seitz notation (Seitz, 1935*b*). It is convenient to use the same symbolism to denote the mapping itself. It will be clear from the context whether $(\mathbf{A}, \mathbf{a})$ denotes the mapping or its representation. The representation $(\mathbf{A}, \mathbf{a})$ can be uniquely decomposed as

$$(\mathbf{A}, \mathbf{a}) = (\mathbf{I}, \mathbf{a})(\mathbf{A}, \mathbf{o}),$$

where $\mathbf{I}$ is the $n\times n$ identity matrix and $\mathbf{o}$ is the $n\times 1$ column consisting entirely of zeros. The pair $(\mathbf{I}, \mathbf{a})$ represents a translation and the column $\mathbf{a}$ is called the translation (or column) part of $(\mathbf{A}, \mathbf{a})$. The pair $(\mathbf{A}, \mathbf{o})$ is a linear transformation and hence leaves the origin fixed. Thus $\mathbf{A}$ is called the linear (or matrix) part of $(\mathbf{A}, \mathbf{a})$. An affine mapping that preserves distances is called an isometry. The group of all isometries, called the Euclidean group $\mathfrak{E}$, is a subgroup of the group $\mathfrak{A}$ of all invertible affine mappings. As space groups are groups of isometries, they are subgroups of $\mathfrak{E}$ (see *IT*, 1987, p. 716).

Let $\mathfrak{G}$ denote a space group. With respect to a primitive basis, each element of $\mathfrak{G}$ can be represented by $(\mathbf{W}, \mathbf{w})$ where $\mathbf{W}$ is a unimodular matrix (see *IT*, 1987, p. 715). Thus, the set of all $\mathbf{W}$'s comprising the linear parts of $\mathfrak{G}$ is a finite unimodular matrix group, *i.e.* a subgroup of $GL(n, \mathbb{Z})$, the group of all unimodular $n\times n$ matrices. This matrix group is a representation of the point group $\mathfrak{P}(\mathfrak{G})$ of $\mathfrak{G}$ (see *IT*, 1987, p. 719). The affine normalizer, $\mathfrak{N}_{\mathfrak{A}}(\mathfrak{G})$, of $\mathfrak{G}$ is defined as follows: an affine mapping $(\mathbf{A}, \mathbf{a})$ is in $\mathfrak{N}_{\mathfrak{A}}(\mathfrak{G})$ if and only if for each $(\mathbf{W}, \mathbf{w})$ in $\mathfrak{G}$ there exists a $(\mathbf{W}', \mathbf{w}')$ in $\mathfrak{G}$ such that

$$(\mathbf{A}, \mathbf{a})(\mathbf{W}, \mathbf{w})(\mathbf{A}, \mathbf{a})^{-1} = (\mathbf{W}', \mathbf{w}'). \quad (2.1)$$

It follows that $\mathfrak{G}$ is a subgroup of $\mathfrak{N}_{\mathfrak{A}}(\mathfrak{G})$. Equation (2.1) can be written as

$$(\mathbf{AWA}^{-1}, \mathbf{a} + \mathbf{Aw} - \mathbf{AWA}^{-1}\mathbf{a}) = (\mathbf{W}', \mathbf{w}')$$

which can be separated into its matrix part

$$\mathbf{AWA}^{-1} = \mathbf{W}' \quad (2.2)$$

and its translation part

$$\mathbf{a} + \mathbf{Aw} - \mathbf{W}'\mathbf{a} = \mathbf{w}'. \quad (2.3)$$

We simplify the task of finding $\mathfrak{N}_{\mathfrak{A}}(\mathfrak{G})$ by dividing the problem into two parts. Since $\mathfrak{G}$ is a subgroup of $\mathfrak{N}_{\mathfrak{A}}(\mathfrak{G})$, there are translations in $\mathfrak{N}_{\mathfrak{A}}(\mathfrak{G})$. These form a normal subgroup of $\mathfrak{N}_{\mathfrak{A}}(\mathfrak{G})$ which is not necessarily discrete but may be continuous in some subspaces. The first part is the determination of this subgroup.

The second part is to find the remaining elements $(\mathbf{A}, \mathbf{a})$ of $\mathfrak{N}_{\mathfrak{A}}(\mathfrak{G})$. In the first step we show that $\mathbf{A}$ must be a unimodular matrix. In the second, we determine which unimodular matrices $\mathbf{A}$ satisfy (2.2). In the third, we find from these matrices $\mathbf{A}$ those for which there exists a column $\mathbf{a}$ such that (2.3) is satisfied. The resulting elements $(\mathbf{A}, \mathbf{a})$ form a set of representatives that, with the translations, completely describes $\mathfrak{N}_{\mathfrak{A}}(\mathfrak{G})$ much as the general positions given in the space-group tables of *IT* (1987) describe $\mathfrak{G}$. Although, in some cases, this list of representatives is infinite, it can always be finitely generated. Such lists of generators are presented in Tables 1 to 4.

The translations of $\mathfrak{N}_{\mathfrak{A}}(\mathfrak{G})$

For a translation of $\mathfrak{N}_{\mathfrak{A}}(\mathfrak{G})$, $\mathbf{A} = \mathbf{I}$, leaving only $\mathbf{a}$ to be determined. Hence (2.2) becomes $\mathbf{W} = \mathbf{W}'$, which does not impose any restrictions on the choice of $\mathbf{a}$. Equation (2.3) becomes

$$\mathbf{a} + \mathbf{w} - \mathbf{Wa} = \mathbf{w}'$$

or

$$(\mathbf{I} - \mathbf{W})\mathbf{a} = \mathbf{w}' - \mathbf{w}.$$

Since $(\mathbf{W}, \mathbf{w})$ and $(\mathbf{W}, \mathbf{w}')$ are elements of $\mathfrak{G}$,

$$(\mathbf{W}, \mathbf{w}')(\mathbf{W}, \mathbf{w})^{-1} = (\mathbf{I}, \mathbf{w}' - \mathbf{w})$$

is a translation in $\mathfrak{G}$. Since the basis is primitive, $\mathbf{w}' - \mathbf{w}$ consists of integers. It follows that

$$(\mathbf{I} - \mathbf{W})\mathbf{a} \in \mathbb{Z}^n \quad \text{for all } \mathbf{W} \in \mathfrak{P}(\mathfrak{G}). \quad (2.4)$$

Suppose that $\mathbf{W}_1$ and $\mathbf{W}_2$ satisfy (2.4). Then there exist $\mathbf{z}_1$ and $\mathbf{z}_2$ in $\mathbb{Z}^n$ such that

$$\mathbf{W}_1\mathbf{a} = \mathbf{a} + \mathbf{z}_1 \quad \text{and} \quad \mathbf{W}_2\mathbf{a} = \mathbf{a} + \mathbf{z}_2$$

and so

$$\mathbf{W}_2\mathbf{W}_1\mathbf{a} = \mathbf{W}_2(\mathbf{a} + \mathbf{z}_1) = \mathbf{a} + \mathbf{z}_2 + \mathbf{W}_2\mathbf{z}_1.$$

Since the entries of $\mathbf{W}_2$ are all integers, $\mathbf{z}_2 + \mathbf{W}_2\mathbf{z}_1$ is in $\mathbb{Z}^n$. Hence, $\mathbf{W}_2\mathbf{W}_1$ satisfies (2.4) whenever $\mathbf{W}_1$ and $\mathbf{W}_2$ satisfy (2.4). Since $\mathfrak{P}(\mathfrak{G})$ is finite, $\mathbf{W}^{-1}$ is a positive power of $\mathbf{W}$, and so it is sufficient to solve (2.4) for a set of generators of $\mathfrak{P}(\mathfrak{G})$.

The set of all $(\mathbf{I}, \mathbf{a})$ satisfying (2.4) can be easily found. As only the matrix parts of $\mathfrak{G}$ occur in (2.4), the result is the same for all space-group types of the same arithmetic crystal class, as is well known [for a definition of arithmetic crystal classes, *cf.* *IT* (1987)].

Example: To find the translations of $\mathfrak{N}_{\mathfrak{A}}(\mathfrak{G})$ for space groups of the arithmetic crystal class $422P$, we use the two generators

$$\mathbf{W}_1 = \begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \text{and} \quad \mathbf{W}_2 = \begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}.$$

Note that the generator (2) of *IT* (1987) is not necessary because it equals $\mathbf{W}_1^2$. We now need to find those columns $\mathbf{a}$ that satisfy (2.4) for $\mathbf{W}_1$ and $\mathbf{W}_2$ simultaneously. For $\mathbf{W}_1$, we have

$$\begin{pmatrix} 1 & 1 & 0 \\ \bar{1} & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = \begin{pmatrix} a_1 + a_2 \\ -a_1 + a_2 \\ 0 \end{pmatrix} = \begin{pmatrix} z_1 \\ z_2 \\ z_3 \end{pmatrix}$$

where z_1, z_2 and z_3 are integers. Hence $a_1 \equiv a_2 \equiv 0, \frac{1}{2} \pmod 1$ and no conditions are placed on a_3. For $\mathbf{W}_2$, we have

$$\begin{pmatrix} 2 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 2 \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = \begin{pmatrix} 2a_1 \\ 0 \\ 2a_3 \end{pmatrix} = \begin{pmatrix} z_1 \\ z_2 \\ z_3 \end{pmatrix}$$

where z_1, z_2 and z_3 are integers. Hence the only additional condition beyond those imposed above is that $a_3 \equiv 0, \frac{1}{2} \pmod 1$. Thus the translations of $\mathfrak{N}_{\mathfrak{A}}(\mathfrak{G})$ for this arithmetic class form a C-centered lattice with $\mathbf{c}' = \frac{1}{2}\mathbf{c}$; (unconventional setting of a conventional P lattice).

The matrix parts of the normalizer $\mathfrak{N}_{\mathfrak{A}}(\mathfrak{G})$

We begin the search for the matrix parts of the normalizers of the space groups by reducing the problem to the realm of point groups. In the same way as the point group $\mathfrak{P}(\mathfrak{G})$ is defined, one defines $\mathfrak{P}[\mathfrak{N}_{\mathfrak{A}}(\mathfrak{G})]$ to be the group consisting of the linear parts of the elements of $\mathfrak{N}_{\mathfrak{A}}(\mathfrak{G})$. We first note that the matrices $\mathbf{A}$ in $\mathfrak{N}_{\mathfrak{A}}(\mathfrak{G})$ are unimodular matrices, *i.e.* elements of $GL(n, \mathbb{Z})$. If $\mathbf{W} = \mathbf{I}$, then, by (2.2), $\mathbf{W}' = \mathbf{I}$. Therefore, $\mathbf{w}$ and $\mathbf{w}'$ in (2.3) are columns of integers and (2.3) reduces to $\mathbf{Aw} = \mathbf{w}'$ for each $\mathbf{A}$. Thus $\mathbf{A} \in GL(n, \mathbb{Z})$.

We now consider the solutions to (2.2). As $\mathbf{W}$ and $\mathbf{W}'$ are elements of $\mathfrak{P}(\mathfrak{G})$ and the solutions of (2.2) are in $GL(n, \mathbb{Z})$, the solutions of (2.2) form the normalizer, $\mathfrak{N}[\mathfrak{P}(\mathfrak{G})]$ in $GL(n, \mathbb{Z})$. Using techniques devised by Brown, Neubüser & Zassenhaus (1973), Brown *et al.* (1978) presented a listing of the generators of the solution sets to (2.2) for the dimensions $n=2$, 3 and 4 in their Tables 5*A*, *B* and *C*, respectively. For dimensions 2 and 3 we checked the entries of these tables by deriving the results by hand in the following way. Again it is sufficient to determine $\mathbf{A}$ for a set of generators of $\mathfrak{P}(\mathfrak{G})$ only.

Example: $\mathfrak{N}_{\mathfrak{A}}(mm2C)$. As generators, we use

$$\mathbf{2}=\begin{pmatrix}\bar{1} & 0 & 0\\ 0 & \bar{1} & 0\\ 0 & 0 & 1\end{pmatrix} \quad \text{and} \quad \mathbf{m}=\begin{pmatrix}0 & 1 & 0\\ 1 & 0 & 0\\ 0 & 0 & 1\end{pmatrix}$$

referred to the primitive basis $\mathbf{a}_p=\frac{1}{2}\mathbf{a}-\frac{1}{2}\mathbf{b}$, $\mathbf{b}_p=\frac{1}{2}\mathbf{a}+\frac{1}{2}\mathbf{b}$, $\mathbf{c}_p=\mathbf{c}$ with respect to the standard basis $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$. We write (2.2) in the form

$$\mathbf{AW}=\mathbf{W}'\mathbf{A}.$$

For $\mathbf{W}=\mathbf{2}$, $\mathbf{W}'$ must equal $\mathbf{2}$ because there is no other rotation. Solving $\mathbf{A2}=\mathbf{2A}$, one obtains

$$\mathbf{A}_{\mathbf{2}p}=\begin{pmatrix}a_{11} & a_{12} & 0\\ a_{21} & a_{22} & 0\\ 0 & 0 & a_{33}\end{pmatrix},$$

where $\det(\mathbf{A}_{\mathbf{2}p})=\pm1$ and the entries are integers. Thus, for example, $a_{33}=\pm1$. Since the matrix representation of $\mathbf{2}$ is the same in the primitive and in the standard bases, the form of $\mathbf{A}_{\mathbf{2}s}$ is the same as that of $\mathbf{A}_{\mathbf{2}p}$. Thus the set $\{\mathbf{A}_{\mathbf{2}p}\}$ of matrices of the form of $\mathbf{A}_{\mathbf{2}p}$ is the normalizer of $112P$.

In $mm2C$, we distinguish the reflections by $\mathbf{m}'$ and $\mathbf{m}$, yielding $m'm2C$. The generator $\mathbf{m}$ may be mapped either onto itself: $\mathbf{Am}=\mathbf{mA}$ or onto $\mathbf{m}'$: $\mathbf{Am}=\mathbf{m}'\mathbf{A}$. In the first case, the solution is

$$\mathbf{A}_{\mathbf{m}p}=\begin{pmatrix}a_{11} & a_{12} & a_{13}\\ a_{12} & a_{11} & a_{13}\\ a_{31} & a_{31} & a_{33}\end{pmatrix}$$

which is the normalizer of $1m1C$ referred to the primitive basis. Transformed to the conventional basis by $\mathbf{A}_{\mathbf{m}s}=\mathbf{B}\mathbf{A}_{\mathbf{m}p}\mathbf{B}^{-1}$ with

$$\mathbf{B}=\begin{pmatrix}\frac{1}{2} & \frac{1}{2} & 0\\ -\frac{1}{2} & \frac{1}{2} & 0\\ 0 & 0 & 1\end{pmatrix},$$

one obtains

$$\mathbf{A}_{\mathbf{m}s}=\begin{pmatrix}a_{11}+a_{12} & 0 & a_{13}\\ 0 & a_{11}-a_{12} & 0\\ 2a_{31} & 0 & a_{33}\end{pmatrix}.$$

Again, since $\mathbf{A}_{\mathbf{m}s}$ is unimodular, $a_{11}-a_{12}=\pm1$, $a_{11}+a_{12}$ and a_{33} must be odd (and $2a_{31}$ is even). This agrees with the form described for $\mathbf{M}_4$ in Table 15.3.3 of *IT* (1987).

In the case $\mathbf{Am}=\mathbf{m}'\mathbf{A}$ the solution is

$$\mathbf{A}_{\mathbf{m}'p}=\begin{pmatrix}a_{11} & a_{12} & a_{13}\\ -a_{12} & -a_{11} & -a_{13}\\ a_{31} & a_{31} & a_{33}\end{pmatrix},$$

$$\mathbf{A}_{\mathbf{m}'s}=\begin{pmatrix}0 & a_{12}-a_{11} & 0\\ -a_{11}-a_{12} & 0 & -a_{13}\\ 2a_{31} & 0 & a_{33}\end{pmatrix}.$$

Combining the conditions of $\mathbf{A}_{\mathbf{2}p}$ with those of $\mathbf{A}_{\mathbf{m}p}$ or $\mathbf{A}_{\mathbf{m}'p}$ and taking into account that $\mathbf{A}$ is unimodular, one obtains

$$\mathbf{A}_{m'm2Cp}=\begin{pmatrix}a_{11} & a_{12} & 0\\ a_{12} & a_{11} & 0\\ 0 & 0 & \pm1\end{pmatrix}$$

or

$$\begin{pmatrix}a_{11} & a_{12} & 0\\ -a_{12} & -a_{11} & 0\\ 0 & 0 & \pm1\end{pmatrix}, \tag{2.5}$$

respectively, where either $a_{11}=0$ and $a_{12}=\pm1$ or $a_{12}=0$ and $a_{11}=\pm1$. Then (2.5) represents $\mathfrak{N}_{\mathfrak{A}}(mm2C)$. There are 16 such matrices which, when defined in terms of an appropriate basis, also represent $4/mmmP$.

The generators found in Brown *et al.* (1978), Table 5*B*, for 2/1/1 ($121P$), 2/2/2 ($1m1C$) and 3/2/2 ($mm2C$) are of the form of (2.5). Conversely, by more extensive calculations, one finds that the generators in Table 5*B* of Brown *et al.* (1978) yield all of the matrices determined by (2.5). Note that the form of $\{\mathbf{A}_{mm2Cs}\}$ is the same as that of $\{\mathbf{A}_{mm2Cp}\}$.

An inversion, as a generator, will not restrict the normalizer because it commutes with any affine mapping. If $\mathfrak{P}(\mathfrak{G})$ is a point group consisting only of proper rotations and the inversion is added as a generator, the normalizer is unchanged. In other cases, however, the inclusion of the inversion may change the normalizer. For example, in $m_xm_y2_z$, the mappings associated with the normalizer must map $\mathbf{2}_z\to\mathbf{2}_z$, and either $\mathbf{m}_y\to\mathbf{m}_x$ or $\mathbf{m}_y\to\mathbf{m}_y$. However, in the case of $2_x/m_x\,2_y/m_y\,2_z/m_z$ there are more combinations to consider, namely the six permutations of $\{\mathbf{2}_x,\mathbf{2}_y,\mathbf{2}_z\}$. Which of these permutations can be realized is partially determined by the arithmetic crystal class and thus by the centering of the lattice. For example, $\mathfrak{N}(mmmI)\gneqq\mathfrak{N}(mm2I)$ but $\mathfrak{N}(mmmC)=\mathfrak{N}(mm2C)$ because, in the latter case, $\mathbf{2}_z$ cannot be mapped onto $\mathbf{2}_x$ or $\mathbf{2}_y$ due to the C centering.

If a point group $\mathfrak{P}(\mathfrak{G})_h$ of higher order has a subgroup $\mathfrak{P}(\mathfrak{G})_l$ of lower order which is characteristic in $\mathfrak{P}(\mathfrak{G})_h$, the normalizer of $\mathfrak{P}(\mathfrak{G})_h$ is a subgroup of that of $\mathfrak{P}(\mathfrak{G})_l$. For example, the cubic point groups have characteristic orthorhombic subgroups. Therefore, their normalizers can be easily obtained from those of the orthorhombic point groups $222P$, $222I$, $222F$, $mmmP$, $mmmI$ and $mmmF$.

A comparison of our hand calculations with the results of Brown *et al.* (1978) revealed that all entries of their Tables 5*A* and *B* were found to be correct except for the normalizer of 2/1/2 (arithmetic crystal class *mc*) appearing in Table 5*A* where the correct entry is 'REP OF 2/2/2' (2*mmc*) instead of the listed entry 'REP OF 2/2/1' (2*mmp*). With this correction, we used the solutions of (2.2) given in these tables.

For a solution $\mathbf{A}$ of (2.2) to be a constituent of some $(\mathbf{A}, \mathbf{a}) \in \mathfrak{N}_{\mathfrak{A}}(\mathfrak{G})$, there must exist an $\mathbf{a}$ satisfying (2.3). Since $\mathfrak{N}_{\mathfrak{A}}(\mathfrak{G})$ is a group, it can be found by determining a set of generators. Moreover, $(\mathbf{A}, \mathbf{a})$ satisfies (2.2) and (2.3) for all elements of $\mathfrak{G}$ if it satisfies these equations for a set of generators $\{(\mathbf{W}, \mathbf{w})\}$ of $\mathfrak{G}$. To show this, suppose that $(\mathbf{W}_1, \mathbf{w}_1)$ and $(\mathbf{W}_2, \mathbf{w}_2)$ satisfy (2.2) and (2.3). Then consider $(\mathbf{W}_2, \mathbf{w}_2)(\mathbf{W}_1, \mathbf{w}_1) = (\mathbf{W}_2\mathbf{W}_1, \mathbf{w}_2 + \mathbf{W}_2\mathbf{w}_1)$. Because $\mathbf{A}(\mathbf{W}_2\mathbf{W}_1)\mathbf{A}^{-1} = (\mathbf{A}\mathbf{W}_2\mathbf{A}^{-1})(\mathbf{A}\mathbf{W}_1\mathbf{A}^{-1}) = \mathbf{W}_2'\mathbf{W}_1'$ we have $(\mathbf{W}_2\mathbf{W}_1)' = \mathbf{W}_2'\mathbf{W}_1'$. By substitution of $\mathbf{w}_2 + \mathbf{W}_2\mathbf{w}_1$, $\mathbf{W}_2'\mathbf{W}_1'$ and $\mathbf{w}_2' + \mathbf{W}_2'\mathbf{w}_1'$ into (2.3), it is straightforward to show that (2.3) is also satisfied by $(\mathbf{W}_2, \mathbf{w}_2)(\mathbf{W}_1, \mathbf{w}_1)$.

For each space group, we applied (2.3) to a set of generating matrices among the solutions of (2.2). For symmorphic space groups, $\mathbf{A}$ satisfying (2.2) has the solution $(\mathbf{A}, \mathbf{o})$ of (2.3) because $\mathbf{w}$ and $\mathbf{w}'$ can always be taken to be zero columns. In other cases, some of the generators $\mathbf{A}$ of (2.2) may not satisfy (2.3) for any $\mathbf{a}$ and so these generators are not in the solution set. When this happens, care must be taken to ensure that the full solution set is found. Let $\mathfrak{U}$ denote the group generated by the generators that satisfy (2.3). If the index of $\mathfrak{U}$ in $\mathfrak{N}[\mathfrak{P}(\mathfrak{G})]$ is a prime number, then $\mathfrak{U} = \mathfrak{P}[\mathfrak{N}_{\mathfrak{A}}(\mathfrak{G})]$ because, in this case, $\mathfrak{U}$ must be a maximal subgroup of $\mathfrak{N}[\mathfrak{P}(\mathfrak{G})]$. Otherwise, $\mathfrak{U}$ might not be maximal, and we looked for the subgroups of $\mathfrak{N}[\mathfrak{P}(\mathfrak{G})]$ which are supergroups of $\mathfrak{U}$ and checked them to find $\mathfrak{P}[\mathfrak{N}_{\mathfrak{A}}(\mathfrak{G})]$. This was done by looking for additional generators to those of $\mathfrak{U}$ not generating the full group $\mathfrak{P}[\mathfrak{N}_{\mathfrak{A}}(\mathfrak{G})]$.

Example. To find the normalizers of space groups $\mathfrak{G}$ equal to $P422$, $P4_122$, $P4_222$ or $P4_322$ (Nos. 89, 91, 93 and 95, respectively), we begin with the translations that we found in the example above, and the point-group normalizer given by Brown *et al.* (1978). Combining these, we obtain $C4/mmm$ (unconventional setting) with $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ referred to the basis of $\mathfrak{G}$. Note that $\mathfrak{G} < \mathfrak{Z} \le \mathfrak{N}_{\mathfrak{A}}(\mathfrak{G}) \le C4/mmm$, with $\mathfrak{Z}$ that *klassengleiche* supergroup of $\mathfrak{G}$ which includes the additional translations as determined above. The group $\mathfrak{Z}$ is called $\mathfrak{K}$ in § 8.3.6 and $\mathfrak{K}(\mathfrak{G})$ in § 15.2 of *IT* (1987). Obviously, index $[C4/mmm: \mathfrak{Z}] = 2$. Consequently, it is sufficient to consider the generator $\bar{1}$.

With $j = 0, \frac{1}{4}, \frac{1}{2}, \frac{3}{4}$, one obtains

$$\begin{pmatrix} \bar{1} & 0 & 0 & | & \alpha \\ 0 & \bar{1} & 0 & | & \beta \\ 0 & 0 & \bar{1} & | & \gamma \end{pmatrix}\begin{pmatrix} 0 & \bar{1} & 0 & | & 0 \\ 1 & 0 & 0 & | & 0 \\ 0 & 0 & 1 & | & j \end{pmatrix}\begin{pmatrix} \bar{1} & 0 & 0 & | & \alpha \\ 0 & \bar{1} & 0 & | & \beta \\ 0 & 0 & \bar{1} & | & \gamma \end{pmatrix}$$

$$= \begin{pmatrix} 0 & \bar{1} & 0 & | & \alpha+\beta \\ 1 & 0 & 0 & | & -\alpha+\beta \\ 0 & 0 & 1 & | & -j \end{pmatrix} = \mathbf{4}'.$$

The matrix $\mathbf{4}'$ represents an element of $\mathfrak{G}$ if and only if $j = 0$ or $\frac{1}{2}$. Hence the normalizers of $P422$ and $P4_222$ contain inversions while those of $P4_122$ and $P4_322$ do not. Therefore, $\mathfrak{N}(P422) = \mathfrak{N}(P4_222) = C4/mmm$ with $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ which is equivalent to $P4/mmm$. The normalizer of $P4_122$ and $P4_322$ is $C4_222$, referred to the basis $\mathbf{a}' = \mathbf{a}$, $\mathbf{b}' = \mathbf{b}$, $\mathbf{c}' = \frac{1}{2}\mathbf{c}$, which is equivalent to $P4_222$.

Example. The normalizer of space group No. 59, *Pmmn*, must obey the equation $Pmmn < \mathfrak{Z} = Pmmm$ $(\mathbf{a}' = \frac{1}{2}\mathbf{a},\ \mathbf{b}' = \frac{1}{2}\mathbf{b},\ \mathbf{c}' = \frac{1}{2}\mathbf{c}) \le \mathfrak{N}_{\mathfrak{A}}(\mathfrak{G}) \le Pm\bar{3}m(\mathbf{a}', \mathbf{b}', \mathbf{c}')$. Choosing as additional generators for $Pm\bar{3}m$

$$\mathbf{3}_d = \begin{pmatrix} 0 & 0 & 1 & | & 0 \\ 1 & 0 & 0 & | & 0 \\ 0 & 1 & 0 & | & 0 \end{pmatrix} \quad \text{and} \quad \mathbf{2}_d = \begin{pmatrix} 0 & 0 & 1 & | & 0 \\ 0 & \bar{1} & 0 & | & 0 \\ 1 & 0 & 0 & | & 0 \end{pmatrix}$$

and for *Pmmn*

$$\mathbf{m}_x = \begin{pmatrix} \bar{1} & 0 & 0 & | & \frac{1}{2} \\ 0 & 1 & 0 & | & 0 \\ 0 & 0 & 1 & | & 0 \end{pmatrix}, \qquad \mathbf{m}_y = \begin{pmatrix} 1 & 0 & 0 & | & 0 \\ 0 & \bar{1} & 0 & | & \frac{1}{2} \\ 0 & 0 & 1 & | & 0 \end{pmatrix},$$

$$\mathbf{m}_z = \begin{pmatrix} 1 & 0 & 0 & | & \frac{1}{2} \\ 0 & 1 & 0 & | & \frac{1}{2} \\ 0 & 0 & \bar{1} & | & 0 \end{pmatrix},$$

one finds that neither $\mathbf{3}_d$ nor $\mathbf{2}_d$ fulfil all of the equations $\mathbf{3}_d m_k \mathbf{3}_d^{-1} = \mathbf{m}_l$ and $\mathbf{2}_d \mathbf{m}_k \mathbf{2}_d^{-1} = \mathbf{m}_l$ with $k = x$, y or z and $l = x$, y or z. However, this does not imply that the crystal class of the normalizer is *mmm*. There remain two cases to be checked: $4_z/mmm$ and $4_x/mmm$ by checking their generators

$$\mathbf{2}_d' = \begin{pmatrix} 0 & 1 & 0 & | & 0 \\ 1 & 0 & 0 & | & 0 \\ 0 & 0 & \bar{1} & | & 0 \end{pmatrix} \quad \text{and} \quad \mathbf{2}_d'' = \begin{pmatrix} \bar{1} & 0 & 0 & | & 0 \\ 0 & 0 & 1 & | & 0 \\ 0 & 1 & 0 & | & 0 \end{pmatrix},$$

respectively. Indeed, $\mathbf{2}_d'$ does satisfy the appropriate equations. Consequently, the normalizer is $P4_z/mmm$ $(\mathbf{a}' = \frac{1}{2}\mathbf{a},\ \mathbf{b}' = \frac{1}{2}\mathbf{b},\ \mathbf{c}' = \frac{1}{2}\mathbf{c})$.

We have determined $\mathfrak{N}_{\mathfrak{A}}(\mathfrak{G})$ for all of the three-dimensional space groups by solving (2.3) for the solutions of (2.2) both by computer and by hand. The affine normalizers of the plane groups have been obtained from the affine normalizers of the space

Table 1. *Affine normalizers of the plane groups p*1 *and p*2: *matrix parts of the non-translation generators*

$$\begin{pmatrix}\bar{1} & 0\\ 0 & \bar{1}\end{pmatrix};\begin{pmatrix}\bar{1} & 0\\ 0 & 1\end{pmatrix};\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix};\begin{pmatrix}1 & 0\\ 1 & 1\end{pmatrix}$$

The vectors of the generating translations are listed in Table 15.3.1 of *IT* (1987, p. 857) under the heading 'Basis vectors'. The column part of each of the non-translation generators is the zero column. For an oblique net, only the first generator represents an isometry; for an accidentally rectangular net, the first two generators represent isometries; for a square net, the first three represent isometries. For the choice of the generators, see text. The first three generators have order 2, the last is of infinite order.

Table 2. *A set of matrix parts of generators of order* 2 *for the affine normalizers of plane groups p*1 *and p*2; *see text*

$$\begin{pmatrix}1 & 0\\ 0 & \bar{1}\end{pmatrix};\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix};\begin{pmatrix}1 & 0\\ 1 & \bar{1}\end{pmatrix}$$

groups by inspection. The Euclidean normalizers of the plane and space groups are obtained by intersecting the affine normalizers with the group of all isometries, *i.e.* by sorting out those mappings which do not leave the quadratic form of the lattice invariant. This is easily done by inspection of the matrix parts in connection with the lattice symmetry. Note that an orthogonal matrix part does not guarantee the mapping to be an isometry. For example, the matrix

$$\begin{pmatrix}-1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 1\end{pmatrix}$$

is orthogonal but is not an isometry of a conventional monoclinic lattice.

Whereas the affine normalizers of all space groups of the same space-group type belong to the same affine type of groups, the Euclidean normalizers depend on the symmetry of the lattice. The Euclidean normalizers listed in the literature are those of space groups for which the lattices correspond to the space-group symmetry (characteristic lattices) and are not accidentally ones of higher symmetry. We have checked the Euclidean normalizers for plane and space groups with characteristic lattices.

3. The results

Employing the method described in the previous section, in 1985 we checked existing lists of normalizers as well as a draft of Tables 15.3.1 to 15.3.4 of *IT* (1987) which had been sent to us for this purpose. In the draft only a typing error had to be corrected. Also, later use of these lists has not brought to light any errors.

The entries of the existing lists of the affine normalizers of plane groups $p1$ and $p2$ and of the triclinic and monoclinic space groups are in the form of matrices with variable entries (*IT*, 1987, Tables 15.3.3 and 15.3.4). The other normalizers are given by sets of generators. We provide generators for the plane groups $p1$ and $p2$ in Tables 1 and 2 and for the triclinic and monoclinic space groups in Tables 3 and 4. In Tables 1 and 3, the generators with orthogonal matrix parts are listed first and are ordered so as to generate

Table 3. *Affine normalizers of the triclinic and monoclinic* (*unique axis b*) *space groups*: *non-translation generators*

$P1$, $P\bar{1}$: (**A**, **o**); (**B**, **o**); (**Z**, **o**); (**C**, **o**); (**D**, **o**); (**E**, **o**)
$P121$, $P12_11$, $P1m1$, $P12/m1$, $P12_1/m1$: (**A**, **o**); (**B**, **o**); (**Z**, **o**); (**D**, **o**); (**E**, **o**)
$P1c1$, $P12/c1$, $P12_1/c1$: (**A**, **o**); (**B**, **o**); (**Z**, **o**); (**E**, **o**); (**F**, **o**)
$C121$, $C1m1$, $C12/m1$: (**A**, **o**); (**B**, **o**); (**Z**, **o**); (**G**, **o**); (**H**, **o**)
$C1c1$, $C12/c1$: (**A**, **o**); (**B**, **o**); (**Z**, **o**); (**G**, **g**); (**H**, **o**)

The matrices **Z**, **A**, **B**, **C**, **D**, **E**, **F**, **G** and **H** as well as the columns **o** and **g** are referred to conventional *IT* coordinate systems, and are listed below. The columns of the generating translations are listed in Table 15.3.2 of *IT* (1987, p. 858) under the heading 'Basis vectors'. For a triclinic lattice, only (**Z**, **o**) represents an isometry. For a monoclinic lattice, only (**Z**, **o**) and (**B**, **o**) represent isometries. For the choice of the generators, see text. Generators **Z**, **A**, **B**, **C** and **D** have orders 2, 2, 2, 3 and 2, respectively; generators **E** to **H** are of infinite order and represent shears.

Matrices:

$$\mathbf{Z}=\begin{pmatrix}\bar{1} & 0 & 0\\ 0 & \bar{1} & 0\\ 0 & 0 & \bar{1}\end{pmatrix};\quad \mathbf{A}=\begin{pmatrix}\bar{1} & 0 & 0\\ 0 & \bar{1} & 0\\ 0 & 0 & 1\end{pmatrix};\quad \mathbf{B}=\begin{pmatrix}\bar{1} & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & \bar{1}\end{pmatrix};\quad \mathbf{C}=\begin{pmatrix}0 & 0 & 1\\ 1 & 0 & 0\\ 0 & 1 & 0\end{pmatrix};$$

$$\mathbf{D}=\begin{pmatrix}0 & 0 & 1\\ 0 & \bar{1} & 0\\ 1 & 0 & 0\end{pmatrix};\quad \mathbf{E}=\begin{pmatrix}1 & 0 & 0\\ 0 & 1 & 0\\ 1 & 0 & 1\end{pmatrix};\quad \mathbf{F}=\begin{pmatrix}1 & 0 & 2\\ 0 & 1 & 0\\ 0 & 0 & 1\end{pmatrix};\quad \mathbf{G}=\begin{pmatrix}1 & 0 & 1\\ 0 & 1 & 0\\ 0 & 0 & 1\end{pmatrix};$$

$$\mathbf{H}=\begin{pmatrix}1 & 0 & 0\\ 0 & 1 & 0\\ 2 & 0 & 1\end{pmatrix};\quad \mathbf{o}=\begin{pmatrix}0\\ 0\\ 0\end{pmatrix};\quad \mathbf{g}=\begin{pmatrix}1/4\\ 1/4\\ 0\end{pmatrix}$$

Table 4. *Generators of finite order for the affine normalizers of the triclinic and monoclinic space groups* (*unique axis b*): *non-translation generators*

$P1$, $P\bar{1}$: (**X**, **o**); (**W**, **o**); (**V**, **o**)
$P121$, $P12_11$, $P1m1$, $P12/m1$, $P12_1/m1$: (**X**, **o**); (**Y**, **o**); (**V**, **o**)
$P1c1$, $P12/c1$, $P12_1/c1$: (**Z**, **o**); (**Y**, **o**); (**U**, **o**); (**S**, **o**)
$C121$, $C1m1$, $C12/m1$: (**Z**, **o**); (**Y**, **o**); (**T**, **o**); (**R**, **o**)
$C1c1$, $C12/c1$: (**Z**, **o**); (**Y**, **o**); (**T**, **g**); (**R**, **g**)

The matrices **Z**, **Y**, **X**, **W**, **V**, **U**, **T**, **S** and **R** as well as the columns **o** and **g** are listed below. The matrices and columns are referred to conventional (*IT*) coordinate systems.

Matrices:

$$\mathbf{Z}=\begin{pmatrix}\bar{1} & 0 & 0\\ 0 & \bar{1} & 0\\ 0 & 0 & \bar{1}\end{pmatrix};\quad \mathbf{Y}=\begin{pmatrix}\bar{1} & 0 & 0\\ 0 & \bar{1} & 0\\ 0 & 0 & 1\end{pmatrix};\quad \mathbf{X}=\begin{pmatrix}0 & 0 & 1\\ 0 & 1 & 0\\ \bar{1} & 0 & 0\end{pmatrix};\quad \mathbf{W}=\begin{pmatrix}0 & 0 & \bar{1}\\ \bar{1} & 0 & 0\\ 0 & \bar{1} & 0\end{pmatrix};$$

$$\mathbf{V}=\begin{pmatrix}0 & 0 & \bar{1}\\ 0 & \bar{1} & 0\\ 1 & 0 & \bar{1}\end{pmatrix};\quad \mathbf{U}=\begin{pmatrix}1 & 0 & 0\\ 0 & 1 & 0\\ 1 & 0 & \bar{1}\end{pmatrix};\quad \mathbf{T}=\begin{pmatrix}1 & 0 & 1\\ 0 & 1 & 0\\ 0 & 0 & \bar{1}\end{pmatrix};\quad \mathbf{S}=\begin{pmatrix}\bar{1} & 0 & 2\\ 0 & 1 & 0\\ \bar{1} & 0 & 1\end{pmatrix};$$

$$\mathbf{R}=\begin{pmatrix}\bar{1} & 0 & \bar{1}\\ 0 & 1 & 0\\ 2 & 0 & 1\end{pmatrix};\quad \mathbf{o}=\begin{pmatrix}0\\ 0\\ 0\end{pmatrix};\quad \mathbf{g}=\begin{pmatrix}1/4\\ 1/4\\ 0\end{pmatrix}$$

The matrices **Z**, **Y**, **U** and **T** have order 2; **X**, **S** and **R** have order 4; **W** and **V** have order 6. For the choice of generators, see text.

the subgroup of all elements of $\mathfrak{N}_{\mathfrak{A}}(\mathfrak{G})$ with orthogonal matrix parts by a composition series. The matrix parts of the remaining one or two generators are 'shear' matrices and hence of infinite order. Following the proposal of a referee, we include Tables 2 and 4 which contain shorter lists of generators. These generators are all of finite order and are only slightly altered from those which the referee kindly provided.

The remarks in the literature on how the normalizers are found generally involve the notion of 'symmetry elements', 'framework of symmetry elements', 'symmetry pattern' *etc.* We have been unable to find a clear definition in these papers of what is meant by these notions nor could we find a comprehensible description of how these concepts can be applied in the derivation of normalizers. However, there must be a procedure by which the normalizers can be obtained by a careful inspection of the space-group diagrams of *IT* or similar tables since these diagrams describe each space group uniquely. Indeed, the first complete list of the Euclidean normalizers of the space groups by Hirshfeld (1968) obtained in this manner is free of errors.

Symmetry elements are frequently used when considering the site symmetries of the atomic positions in crystal structures or of Wyckoff positions. Here, they are sets of fixed points together with some information on the operations involved with these fixed points. Even this simple concept of symmetry element is sufficient to derive the normalizers of many space groups. There are space groups, however, where it fails. For example, in $P1m1$ the pattern of symmetry elements would consist of a set of parallel and equidistant mirror planes. The symmetry of this pattern contains all rotations about any axis perpendicular to these planes including the non-crystallographic ones. However, the linear part of any element in the Euclidean normalizer must be crystallographic since it maps the lattice onto itself. Thus, in this example, the Euclidean normalizer is a proper subgroup of the symmetry group of this symmetry pattern. Consequently, to determine whether an isometry is in the normalizer of a space group, the condition that its linear part maps the lattice of the space group onto itself, see *e.g.* Hirshfeld (1968), has to be satisfied. Moreover, in some cases of enantiomorphic space groups, the handedness of the screw axes is essential.

We suppose that such a procedure for deriving the normalizers of space groups may be designed using the rigorous definition of 'symmetry element' which has recently been published by de Wolff *et al.* (1989). We have not tried to establish this procedure. Instead of such a visual approach, we prefer the matrix method provided above. It has the advantage of (i) not depending on the availability of diagrams, (ii) being adaptable to the use of a computer, and (iii) being independent of the dimension of space, at least in principle.

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References

BILLIET, Y., BURZLAFF, H. & ZIMMERMANN, H. (1982). *Z. Kristallogr.* **160**, 155-157.

BROWN, H., BÜLOW, R., NEUBÜSER, J., WONDRATSCHEK, H. & ZASSENHAUS, H. (1978). *Crystallographic Groups of Four-Dimensional Space.* New York: Wiley.

BROWN, H., NEUBÜSER, J. & ZASSENHAUS, H. (1973). *Math. Comput.* **27**, 167-182.

BURZLAFF, H. & ZIMMERMANN, H. (1980). *Z. Kristallogr.* **153**, 151-179.

DZYABCHENKO, A. V. (1983). *Acta Cryst.* A**39**, 941-946.

DZYABCHENKO, A. V. (1986). In *Group Theoretical Methods in Physics. Proc. Third Yurmala Seminar,* 1985. Utrecht: VNU Science Press.

FISCHER, W. (1968). *Acta Cryst.* A**24**, 67-81.

FISCHER, W. (1971). *Z. Kristallogr.* **133**, 18-42.

FISCHER, W. & KOCH, E. (1983). *Acta Cryst.* A**39**, 907-915.

GALIULIN, R. V. (1978). *Sov. Phys. Crystallogr.* **23**, 635-641.

GALIULIN, R. V., NARDOV, A. V., SHUSTOV, A. V. & DELONE, B. N. (1976). *Sov. Phys. Dokl.* **21**, 614-615.

GIACOVAZZO, C. (1980). *Direct Methods in Crystallography.* London: Academic Press.

GREUB, W. (1975). *Linear Algebra,* 4th ed. New York: Springer.

GUBLER, M. (1982*a*). *Uber die Symmetrien der Symmetriegruppen: Automorphismengruppen, Normalisatorgruppen und charakteristische Untergruppen von Symmetriegruppen, insbesondere der kristallographischen Punkt- und Raumgruppen.* Dissertation. Zürich Univ., Switzerland.

GUBLER, M. (1982*b*). *Z. Kristallogr.* **158**, 1-26.

HAUPTMAN, H. & KARLE, J. (1953). *Solution of the Phase Problem. I. The Centrosymmetric Crystal. Am. Crystallogr. Assoc. Monogr.* No. 3.

HAUPTMAN, H. & KARLE, J. (1956). *Acta Cryst.* **9**, 45-55.

HAUPTMAN, H. & KARLE, J. (1959). *Acta Cryst.* **12**, 93-97.

HIRSHFELD, F. L. (1968). *Acta Cryst.* A**24**, 301-311.

Internationale Tabellen zur Bestimmung von Kristallstrukturen (1935). Bd. I. Leipzig: Borntraeger.

International Tables for Crystallography (1983). Vol. A. Dordrecht: Reidel. (Present distributor Kluwer Academic Publishers, Dordrecht.)

International Tables for Crystallography (1987). Vol. A, 2nd ed. Dordrecht: Reidel. (Present distributor Kluwer Academic Publishers, Dordrecht.)

International Tables for X-ray Crystallography, (1952). Vol. I. Birmingham: Kynoch Press.

International Tables for X-ray Crystallography (1974). Vol. IV. Section 6.1: *Origin specification,* pp. 339-349. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)

KARLE, J. & HAUPTMAN, H. (1961). *Acta Cryst.* **14**, 217-223.

KOCH, E. & FISCHER, W. (1975). *Acta Cryst.* A**31**, 88-95.

PARTHÉ, E. & GELATO, L. M. (1984). *Acta Cryst.* A**40**, 169-183.

SAYARI, A. & BILLIET, Y. (1977). *Acta Cryst.* A33, 985-986.
SAYARI, A., BILLIET, Y. & ZARROUK, H. (1978). *Acta Cryst.* A34, 553-555.
SEITZ, F. (1935*a*). *Z. Kristallogr.* 90, 289-313.
SEITZ, F. (1935*b*). *Z. Kristallogr.* 91, 336-366.
WOLFF, P. M. DE, BILLIET, Y., DONNAY, J. D. H., FISCHER, W., GALIULIN, R. B., GLAZER, A. M., SENECHAL, M., SHOEMAKER, D. P., WONDRATSCHEK, H., HAHN, TH., WILSON, A. J. C. & ABRAHAMS, S. C. (1989). *Acta Cryst.* A45, 494-499.

Acta Cryst. (1990). A46, 552-559

Intensity Distributions in Fiber Diffraction

BY R. P. MILLANE

The Whistler Center for Carbohydrate Research, Smith Hall, Purdue University, West Lafayette, Indiana 47907, *USA*

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Abstract

The probability distributions of X-ray intensities in fiber diffraction are different from those for single crystals (Wilson statistics) because of the cylindrical averaging of the diffraction data. Stubbs [*Acta Cryst.* (1989), A45, 254-258] has recently determined the intensity distributions on a fiber diffraction pattern for a fixed number of overlapping Fourier-Bessel terms. Some properties of the amplitude and intensity distributions are derived here. It is shown that the amplitudes and intensities are approximately normally distributed (the distributions being asymptotically normal with increasing number of Fourier-Bessel terms). Improved approximations using an Edgeworth series are derived. Other statistical properties and some asymptotic expansions are also derived, and normalization of fiber diffraction amplitudes is discussed. The accuracies of the normal approximations are illustrated for particular fiber structures, and possible applications of intensity statistics in fiber diffraction are discussed.

Notation

$\mathcal{G}\ (\mathcal{I})$	amplitude (intensity) on a fiber diffraction pattern.
$\mathcal{E}$	normalized amplitude.
m	number of degrees of freedom for $\mathcal{G}$.
$P_m(\mathcal{G}),\ P_m(\mathcal{I})$	probability density functions for $\mathcal{G}$ and $\mathcal{I}$.
$\alpha_{mn}\ (\beta_{mn})$	nth moment of $\mathcal{G}\ (\mathcal{I})$.
$\mu_m\ (\nu_m)$	mean of $\mathcal{G}\ (\mathcal{I})$.
$\sigma_m^2\ (\tau_m^2)$	variance of $\mathcal{G}\ (\mathcal{I})$.
$\mu_{mn}\ (\nu_{mn})$	nth central moment of $\mathcal{G}\ (\mathcal{I})$.
$Q_m(\mathcal{G}),\ Q_m(\mathcal{I})$	cumulative distribution functions for $\mathcal{G}$ and $\mathcal{I}$.
$\varphi_m(y),\ \psi_m(y)$	characteristic functions for $\mathcal{G}$ and $\mathcal{I}$.
κ_{mn}	nth cumulant for $\mathcal{I}$.
$\hat{P}_m(\mathcal{G}),\ \hat{P}'_m(\mathcal{G}),\ \hat{P}_m(\mathcal{I})$	normal approximations to $P_m(\mathcal{G})$ and $P_m(\mathcal{I})$.
$\tilde{P}_m(\mathcal{G}),\ \tilde{P}'_m(\mathcal{G}),\ \tilde{P}_m(\mathcal{I})$	Edgeworth series approximations to $P_m(\mathcal{G})$ and $P_m(\mathcal{I})$.
$\hat{Q}_m(\mathcal{G}),\ \hat{Q}'_m(\mathcal{G}),\ \hat{Q}_m(\mathcal{I})$	normal approximations to $Q_m(\mathcal{G})$ and $Q_m(\mathcal{I})$.
$\hat{\varphi}_m(y),\ \hat{\psi}_m(y)$	normal approximations to $\varphi_m(y)$ and $\psi_m(y)$.

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1. Introduction

Statistical descriptions of X-ray amplitudes have played important roles in many aspects of crystallography. The most remarkable, of course, is the use of conditional distributions of phases in direct methods for phase determination (Hauptman & Karle, 1953; Giacovazzo, 1980; Bricogne, 1984). Other applications include detection of symmetry (Wilson, 1949), analysis of twinning (Yeates, 1988), and estimation of R factors (Wilson, 1950; Luzatti, 1952). The initial application of such ideas was a study of the distribution of intensities diffracted by a crystal (Wilson, 1949).

X-ray fiber diffraction is a variant of traditional crystallography that can be used to determine structures of molecules that prefer to form fibers rather than single crystals (Millane, 1988). In a fiber specimen, the diffracting particles are randomly rotated so that the diffraction pattern is cylindrically averaged. Intensity distributions in fiber diffraction are therefore different from those in traditional crystallography. Although intensity statistics have not yet been utilized in fiber diffraction, it may be possible to develop useful applications. The first step in this