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Classification of Symmetry Groups

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(*Received* 18 *October* 1960 *and in revised form* 19 *December* 1960)

Point groups and space groups in 3-D are two classes of symmetry groups that have proved most useful in crystallography. Recently other sorts of groups have been described involving a change of 'side', sign (antisymmetry), or color; and some of these have already been applied to problems of twinning and magnetic structures. A uniform classification of these various groups should help in visualizing the relations among them and in working out new applications.

If all variables are treated geometrically, including antisymmetry, symmetry groups may be classed according to the dimensions of space that are invariant under their operations. Thus the 80 'antisymmetry groups in a plane' have 2-D and 3-D spaces invariant. The group is 'in' the highest dimensional space of invariance, and translations are allowed only in the lowest dimensional space. But spaces of intermediate dimensions may also be invariant: the 31 'Streifenornamente' have 1, 2, 3 spaces invariant. Alternatively these classes may be described by the symmetry of the invariant space, using the continuous translations and rotations. Thus the class of groups in 2, 3 space are all the crystallographic subgroups of $t\infty/mm$, and class 1, 2, 3 are all subgroups of $\mathbf{t}mmm$.

All such classes through 4-D are tabulated.

Introduction

After the classical descriptions of crystallographic lattices and space groups in the nineteenth century, it was generally considered that everything had been said on the subject. There was a revival of interest about 1930 when several papers appeared in the *Zeitschrift für Kristallographie* describing line groups, plane groups, three-dimensional groups in four dimensions, continuous groups, and so on. These esoteric matters were soon forgotten, but ever since the appearance in 1951 of Schubnikov's book on antisymmetric point groups, the field has blossomed. Antisymmetry is a beautifully simple idea that has moreover proved useful in solving magnetic structures and other problems. Symmetry groups are now generally classified in terms of antisymmetry or extensions of that idea (Zamorzaev & Sokolov, 1957; Mackay, 1957; Niggli, 1959; Nowacki, 1960). It is the single purpose of this paper to recall and develop another aspect of symmetry groups that can serve as a basis of classification. I refer to the space—point, plane, line, cell, or some combination of them—that is invariant under all operations of the symmetry groups in a class. The dimensions of the space, or its general symmetry, is a description of the class of groups. With this alternate viewpoint, groups are more easily described for some purposes.

Antisymmetry and dimensions

I take as point of departure the paper by Heesch (1930*a*), 'Über die vierdimensionalen Gruppen des dreidimensionalen Raumes'. These groups are in fact the antisymmetric or black and white groups in 3-D, now generally known as the Schubnikov groups. A point can be described in 3-D by the coordinates x, y, z; then whereas Heesch gives it values of plus or minus w in a fourth dimension, Schubnikov and Belov label it black or white.* Antisymmetry is equivalent to a bivalued function in an added dimension. How far, and to what purpose, can this aspect of groups be developed?

Dimensional classification of symmetry groups

The dimensional relations of symmetry groups are most easily appreciated in few dimensions. The 80 antisymmetric plane groups (Belov, Nerenova & Smirnova, 1955; Mackay, 1957, p. 544) can also be called 2-D (plane)groups in three dimensions (Heesch, 1930*a*, p. 326). Niggli (1959, p. 300) lists them both ways: (1) as 80 symmetry groups with 2-D translation in 3-D space (Schichtgruppen G_3^2) and (2) as 46 antisymmetry groups with 2-D translation in 2-D space ($G_2^{2\prime}$) (plus 17 'black' or one-sided groups, and 17 'gray' or mirrored groups, equals 80). He apparently does not think it necessary to point out this equivalence (or two other similar equivalences) that occur in his table.

It is important to remember that points anywhere in 3-D space, however far they may be from the reference plane, can be related by these 80 2-D groups. The reference plane imposes only two restrictions: (1) it is the locus of all translations, and (2) it is invariant under all rotations and reflections. The first of these is used by Niggli (1959) as a basis for his classification. But there can be more than one class of groups with the same translational elements. Consider the groups with translation along only a single reference line. If points only on the line are allowed, there are two such groups (*International Tables for X-ray Crystallography*, Vol. I, p. 45). If points are also allowed in a plane (that contains the line), it is well known that there are 7 such groups (*International Tables for X-ray Crystallography*, Vol. I, p. 56). Now if we retain the reference line and plane, and allow points anywhere in 3-D space, 31 symmetry groups are possible. Speiser first described these as 'Streifenornamente', in terms of the symmetry of a strip ornament that has relief (Speiser, 1956, p. 81–86). On the other hand, these are also antisymmetry groups with 1-D translation in 2-D space (Belov, 1956, p. 475; Niggli, 1959: $17G_2^{1\prime}$ groups, plus 7 'black' and 7 'gray' groups equals 31). But when we consider the point groups (I count 16) that are isomorphous with these 31 groups, we find they have no place in the classifications of Niggli or Mackay (1957). Similar troubles will be found with the groups involving 2-D translations.

However, these classes of groups are distinguished in a straightforward manner by the second restriction that was mentioned above, that is, in terms of the line or plane that is invariant under rotations and reflections. By invariance I mean that any symmetry operation of the group acts on the line or plane to give it back unchanged. Actually both restrictions can be stated in these terms, when you realize that if a plane is the locus of all translations, it is invariant with such translations. So both restrictions can be combined by saying that the plane or line is invariant under *all* symmetry operations of that class of groups. Then if several dimensional descriptions are involved, such as a plane and a line in the 7 groups mentioned above, translation is necessarily restricted to the *lowest* dimension of invariance (1-D). Analogously, point groups have zero as their lowest dimension. Furthermore, if a group is 'in' 2-D space, 2-D space must be invariant with respect to that group. This is the *highest* dimension of invariance. From this viewpoint all the classes of groups mentioned in the preceding paragraph may be designated in terms of their dimensional invariance: 80 groups of class 2, 3; 2 groups of class 1; 7 groups of class 1, 2; 31 groups of class 1, 2, 3; and 16 groups of class 0, 1, 2, 3.

The classes of groups up to 3-D are listed in Table 1 according to this 'dimensional' description. In the second and third columns of Fig. 1 these dimensions are represented graphically. All the dimensions listed are invariant with respect to any group in that class; the group lies in the space of highest dimension, and has translation along the lowest dimension.* If desired, the list of dimensions may be considered a symbol of the class of groups. Please understand that Fig. 1 is schematic, and while the boundaries of each space have been drawn to conform with its symmetry (see below), the space in which symmetry may operate actually extends infinitely in one or more directions. The equivalence of classes 0, 1, 3 and 0, 2, 3 will be discussed in the following section.

This sort of description has perhaps some advantage of being mathematically consistent and explicit, in recognizing that all coordinates of a point can be expressed geometrically. Any of these dimensions may or may not correspond to dimensions of real space. Where all the dimensions *do* correspond to real space, as in the application to twinning theory, of groups of kinds 2, 3, and 0, 2, 3 (Holser, 1957) and 1, 2, 3, and 0, 1, 2, 3 (Holser, 1960), the full dimensional description has obvious advantages. Even where one of the coordinates is chemical composition (Heesch, 1930, p. 341–342) or magnetic spin (Donnay *et al.*, 1958), it at least serves to remind us that a coordinate may have any value so long as the symmetry is satisfied. The space is not bounded by two lines (or planes),

* Although Schubnikov in his book (1951) makes no mention of Heesch (1930*a*), the latter had already described the 122 antisymmetric point groups and many of the corresponding space groups.

* Isomorphic groups can be constructed with fewer than this maximum permitted number of dimensions of translation (Schubnikov, 1929).

Table 1. *Some classes of symmetry groups in* 3-D

Invariance: Dimensional	Invariance: Symmetrical	Number of groups*	Other notations
0	1	1	G_0^0 (Niggli, 1959)
0, 1	*m*	2	Eindimensionaie Punktgruppen G_1^0, $G_0^{0\prime}$ (Niggli, 1959)
0, 1, 2	*mm*	5	$G_1^{0\prime}$ (Niggli, 1950); eindimensionale 'zweifarbige' Kristallklassen (Nowacki, 1960, p. 97)†
0, 1, 2, 3	*mmm*	16	Bordürenmuster Klassen (Nowacki, 1960, p. 97)‡
0, 1, 3 } 0, 2, 3 }	∞/mm	31	Black and white point groups in 2-D (Mackay, 1957): $G_2^{1\prime}$ (Niggli, 1959)
0, 2	$\infty\, m$	10	Identity point groups in 2-D (Mackay, 1957); zweidimensionale Punktgruppen G_2^0 (Niggli, 1959)
0, 3	$\infty/m\,\infty$	32	Point groups; identity point groups in 3-D (Mackay, 1957); dreidimensionale Punktgruppen G_3^0 (Niggli, 1959)
1	$\mathbf{t}m$	2	1-D space groups (*International Tables for X-ray Crystallography*, 1952, p. 45), Reihengruppen G_1^1 (Niggli, 1959)
1, 2	$\mathbf{t}mm$	7	Bortenornamente (Speiser, 1956, p. 81); line groups in 2-D (*International Tables for X-ray Crystallography*, 1952, p. 56); odnomernye odnostoronnie beskonechnyi gruppy (Belov, 1956); Bandgruppen G_2^1, $G_1^{1\prime}$ (Niggli, 1959); eindimensionale 'zweifarbige' Gruppen (Nowacki, 1960, p. 97†)
1, 2, 3	$\mathbf{t}mmm$	31	Streifenornamente (Speiser, 1956, p. 83); odnomernye drustoronnie beskonechnye gruppy (Belov, 1956); $G_2^{1\prime}$ (Niggli, 1959)
1, 3	$\mathbf{t}\,\infty/mm$	75	Kettengruppen (Hermann, 1929); line groups in 3-D (*International Tables for X-ray Crystallography*, 1952, p. 56), Balkengruppen G_3^1, $G_1^{1\prime}$ (Niggli, 1959)
2	$t\,\infty\, m$	17	Flächengruppen (Niggli, 1924); 2-D space groups (*International Tables for X-ray Crystallography*, 1952, p. 45); ploskie odnostoronnie gruppy (Belov & Tarkhova, 1956); identity space groups in 2-D (Mackay, 1957); Flächengruppen G_2^2 (Niggli, 1959)
2, 3	$t\,\infty/mm$	80	Netzgruppen (Hermann, 1929); zweidimensionale Raumgruppen (Alexander & Hermann, 1929); ploskie dvukhtsvetnie gruppy (Belov & Tarkhova, 1956; Belov, 1959); black and white space groups in 2-D (Mackay, 1957); Schichtgruppen G_3^2, $G_2^{2\prime}$ (Niggli, 1959)
3	$T\,\infty/m\,\infty$	230	Raumgruppen (Schoenflies); space groups; federovskie gruppy (Belov & Tarkhova, 1956)

* Including trivial cases, and with the lattice 'crystallographic' restriction.
† Nowacki counts 4 groups of class 0, 1, 2 and 6 groups of class 1, 2, leaving out *mm* (*pi'i* in his notation).
‡ Nowacki counts 9 groups of class 0, 1, 2, 3: leaving out the 'gray' groups $112/m$, $12/m1$, $2mm$, and *mmm*, and also in three cases equating groups that differ only in the orientation of symmetry elements relative to the line (See also Holser, 1960, p. 26.)

as Speiser (1956, p. 83) and Niggli (1953, p. 63) imply. A 'black and white' group can also describe the relations of 'red and green' in the same space, if the relations of black, white, red, and green along a single coordinate can be stated or assumed.

The dimensional description has the disadvantage of requiring an additional dimension for visualization of the relations, and this may be troublesome if four or more dimensions are involved. Classes of 4-D groups are listed in Table 2.

Symmetry of Invariance

If a plane is invariant with respect to a particular symmetry operation, that is another way of saying that the operation is a symmetry element of the plane. This indicates that the essential feature of the plane in its relation to symmetry groups is not so much that it has two dimensions, but that it has a certain symmetry. The symmetry of an infinite plane is defined by a continuous group, that is, one whose translational components are infinitesimal (Schubnikov, 1929; Heesch, 1930*b*). Schubnikov's notation can be modified to conform with that of the *International Tables for X-ray Crystallography* (1952) by using the symbols **t**, *t* and *T* for continuous (infinitesimal) translations in 1-D, 2-D, and 3-D, respectively, and ∞ for continuous (infinitesimal) rotations. The symbol for plane symmetry in 2-D (class 2) is then $t\infty 2/m$, in which the symbols have the following significance:

- *t* is a set of continuous translations that cover the plane,
- ∞ is a continuous rotation axis perpendicular to the plane (which is multiplied infinitely by *t*),
- 2 is a 2-fold axis lying in the plane (which is multiplied infinitely in direction by ∞, and infinitely in position by *t*),
- *m* is a mirror plane perpendicular to 2 (for every one of the double infinity of 2 axes).

Part of the symbol is redundant, and it may therefore be shortened in the usual way to $t\infty m$.

The class of groups with respect to each of which a plane is invariant, is the class of all subgroups of

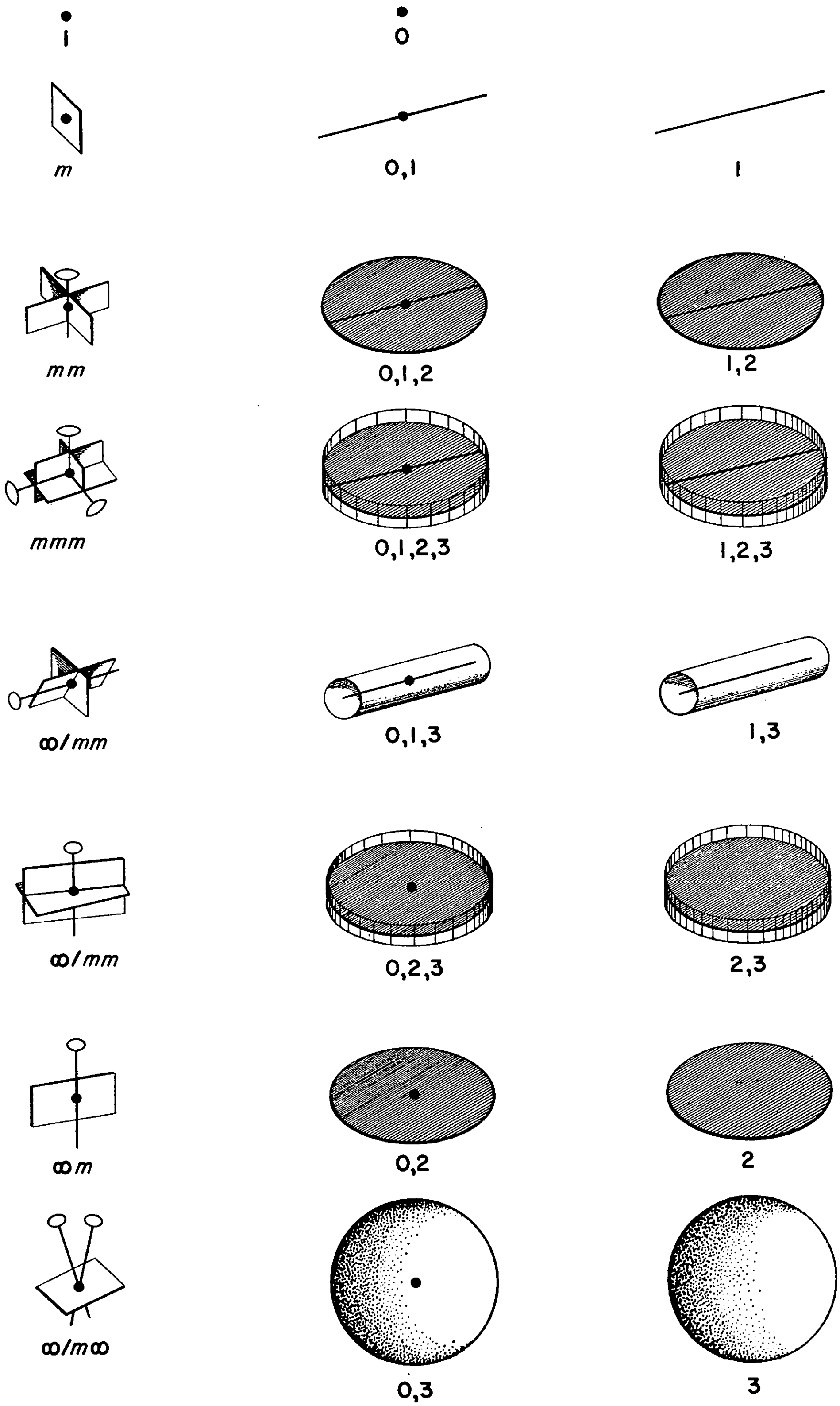

Fig. 1. Schematic representation of the dimensions invariant for each of the classes of groups up to 3-D are shown on the right, and on the left the corresponding symmetry for the point (0) classes.

Table 2. *Some additional classes of symmetry groups in* 4-D

Invariance: Dimensional	Invariance: Symmetrical*	Number of groups†	Other notations
0, 4	$\infty' \infty' \infty''$	122?	Identity point groups in 4-D (Mackay, 1957)
0, 1, 4 0, 3, 4	$(\infty' \infty')m$	122	Vierdimensionalen Punktgruppen des dreidimensionalen Raumes (Heesch, 1930); gruppy antisimmetrii konechnikh figur (Schuknikov, 1951); black and white point groups in 3-D (Mackay, 1957)†; $G_3^{0'}$ (Niggli, 1959)
0, 2, 4	$(\infty m)(\infty m)\infty'' = (\infty m)(\infty m)$	8	$G_2^{0''}$ (Niggli, 1959)
0, 1, 2, 4 0, 1, 3, 4 0, 2, 3, 4	$(\infty\ m)mm = (\infty'\ m)m$	?	Tensor field black and white point groups in 2-D, $n=2$ (Mackay, 1957)
0. 1, 2, 3, 4	$mmmm$	?	Tensor field black and white point groups in 1-D, $n=3$, in Mackay's (1957) nomenclature
1, 4	$\mathbf{t}(\infty' \infty')m$	?	
1, 2, 4 1, 3, 4	$\mathbf{t}(\infty'\ m)m$	?	$G_3^{1'}$, $G_2^{1''}$ (Niggli, 1959)
1, 2, 3, 4	$\mathbf{t}mmmm$	?	Tensor field black and white space groups in 1-D, $n=3$, in Mackay's (1957) nomenclature
2, 4	$t(\infty m)(\infty m)$	95 (= 80 + 15)	Gruppy tsvetnoi symmetrii (Belov & Tarkhova, 1956); colour space groups (Mackay, 1957); $G_2^{2''}$ (Niggli, 1959)
2, 3, 4	$t(\infty' m)m$	173	Tensor field black and white space groups in 2-D, $n=2$ (Mackay, 1957); $G_3^{2'}$ (Niggli, 1959)
3, 4	$T(\infty' \infty')m$	1651	Vierdimensionalen Raumgruppen des dreidimensionalen Raumes (Heesch, 1930); schubnikovskaie gruppy (Belov, Nerenova & Smirnova, 1955); black and white space groups in 3-D (Mackay, 1957); $G_3^{3'}$ (Niggli, 1959)
4	$\mathbf{T}\ \infty' \infty' \infty''$	?	Identity space groups in 4-D (Mackay, 1957)

* See Appendix, and Table 3.
† Including trivial cases and with the lattice 'crystallographic' restriction.
‡ Mackay lists 129 groups of class 0, 1, 4: perhaps this has been exchanged with class 0, 4 by a printer's error.

Note added in proof: I now find that Hurley [(1951) *Proc. Cambridge Phil. Soc.* **47**, 650] counted 222 groups of class 0,4; and Pabst [(1961) *Amer. Cryst. Assn. Denver Meeting Abstracts*] has counted 179 groups of class 1, 2, 3, 4.

$t\infty m$. Or, the crystallographic plane groups of class 2 in Table 1, are all the subgroups of $t\infty m$ that are crystallographically permitted. The continuous translation t gives any 2-D lattice as a suboperation; and ∞ gives any rotational operation. The symbol may be used to designate either the symmetry of the plane itself, or the class of groups related to it, as determined by the context. If the class includes non-crystallographic groups, such as those involving continuous rotations, the class will cover all symmetries of aggregates ('textures' of Schubnikov (1955)).

A further example may clarify the nomenclature of symmetry. The 31 groups of class 1, 2, 3 that were discussed previously have the general supergroup symmetry $\mathbf{t}2/m2/m2/m$ (= $\mathbf{t}mmm$), the m's referring to reflection along the line, along the plane perpendicular to the line, and perpendicular to line and plane, respectively. The last of these mirrors is in real space in a relief ornament or a twin, in 'color space' for a two-color strip ornament or other antisymmetric figure. Analogously, both the second and third mirrors can be in non-geometrical space. But none of these variations affect the essential nature of the group, or their classification by invariance of dimensions or symmetry. The corresponding 16 groups of class 0, 1, 2, 3 have a symmetry mmm, as shown in Fig. 1.

Column 2 of Table 1 lists the symmetry symbols for the various classes of crystallographic groups up to 3-D, and the 'point symmetries' (0 classes) are illustrated in Fig. 1. This system can be extended to 4-D, with perhaps somewhat less usefulness, as shown in the second column of Table 2. Symmetry operations for 4-D, and their notation, are discussed in an Appendix.

Five or more dimensions would be required for the more complex generalizations of space groups: if plus and minus (or black and white) are associated with n tensor components (Mackay, 1957; equivalent to the l sign changes of Zamorzaev & Sokolov, 1957; Zamorzaev, 1958) in N dimensions, each corresponds to a reflection along a new dimension. A total of $N+n$ dimensions are then required for the symmetrical representation. Note that the possible symmetry operations in the new dimensions are not exhausted by this reflection. In two added dimensions rotation is possible, equivalent to the 'color groups' of Belov & Tarkhova (1956) or the 'Entartungssymmetrie' of Niggli (1959). Among three added dimensions rotary inversion ('colored', if you like) is possible, and so on. These rotations are one point symmetry, so the number of extra dimensions required for representation can sometimes be reduced by one, by mapping the rotation element of dimensions n into a periodic lattice of dimensions $n-1$ (Coxeter, 1947, p. 236). Thus the rotation in the 'color' plane, of groups $t\ (\infty m)\ (\infty m)$ of Table 2, corresponds to the periodic translation component of the 3-D screw axes used by Belov & Tarkhova (1956) in *their* derivation of the plane color groups.

The classification in terms of symmetry rather than in terms of dimensions calls attention to the fact that '2-D point groups in a plane' (dimensional class 0, 2, 3) and '3-D point groups on a line' (dimensional class 0, 1, 3) are really the same 31 point groups—both geometrical restrictions have the same symmetry $\infty/m2/m$.* Other equivalences are found in 4-D (Table 2). If the maximum and minimum dimensions of invariance are m and n, then the number of dimensional classes is 2^{m-n}, but this number is reduced by the symmetrical equivalences.

It also suggests that *any* group can serve as a basis for a class of groups consisting of its subgroups. The other point groups with infinite rotations are (Schubnikov, 1951, p. 78): ∞, ∞/m, $\infty/2$, $\infty\infty$. With a little strain these can also be visualized in terms analogous to the dimensional classifications; for example symmetry ∞ corresponds to a plane in which rotations are permitted in only one sense, or a line along which a screw axis is permitted in only one sense All but ∞/m are enantiomorphous. These classes of point groups correspond to the 'types' of Schubnikov (1959). Analogous groups with continuous translations in 1-, 2-, 3-, or even 4-D may be constructed. Of course any crystallographic group, in addition to the four listed above (1, m, $2mm$, mmm), can also serve as the basis for a class of groups: its subgroups.

* Note that these are not the same as the line groups of class 1, 2, 3 (symmetry $2/m2/m2/m$) that were discussed above; the latter also number 31 only by coincidence. Also, of course, it is not analogously true that class 2, 3 and 1, 3 are the same; these have symmetries $t\infty/m2/m$ and $\mathbf{t}\,\infty/m2/m$, and number 80 and 75 respectively.

APPENDIX

Symmetri operations in 4-D

Symmetry operations and groups in 4-D have been discussed by Motzok (1930), Coxeter (1947) and Hermann (1949), but unfortunately with differing viewpoints and notations. The possible types of symmetry operations in 4-D are listed in Table 3. The operations that are new to this dimension are: di-rotations (no translation involved), and rotary-inversion-glide (or roto-reflection-glide). The corresponding elements of symmetry are a point and a line, respectively, and other elements of symmetry have one more dimension than their corresponding elements in 3-D (rotation is around a plane, reflection is through 3-D 'cell', etc.). Coxeter (1947, p. 75) treats all symmetry in terms of reflections, and has no notation analogous to those of Table 3.

Continuous rotations and rotary inversions are logically designated by ∞, and ∞', respectively. Continuous di-rotations are designated by ∞'', following Niggli's (1959) notation for *Entartungssymmetrie*, although not all di-rotations have an equivalent among the *Entartungssymmetrie* operations of Niggli (1959). Hermann's short notation (column 3 of Table 3) might have been more rigorous, but less recognizable.

The only published notation (Coxeter, 1934; 1947, p. 69) for 4-D groups uses Schlafli symbols, which describe morphology and topology, not just the symmetry. Rather than construct a complete system analogous to that of the *International Tables for X-ray Crystallography*, a brief notation sufficient for Table 2 was devised from the following considerations. The symmetry of the 4-D hypersphere can be adequately represented by adding a continuous di-rotation to the

Table 3. *Types of symmetry operations in* 4-D

	Discontinuous operations			Corresponding antisymmetry (Belov, Neronova & Tarkhova, 1954; Niggli, 1959)	Continuous Operations (this paper)
Motzok, 1930		Hermann, 1949 Long (p. 141–144)	Hermann, 1949 Short (p. 145)		
Identitat	1	1111	—	1	(1)
Reflexion	P	2111	2_{000}	$1'=m$	(m)
Rotation	L_2 $L_3, \ldots$	2211 311, . . .	2_{00} $3_{00}, \ldots$	m' 3, . . .	∞
Roto-reflection	P $P_6^6, \ldots$	2221 321, . . .	2_0 $3_0, \ldots$	$2'$ $3', \ldots$	$\infty' \equiv \infty/m$
Di-rotation	$L_{2\cdot 2}$ $L_{6\cdot 2}, \ldots$ $L_{3\cdot 3}, \ldots$	2222 322, . . . 33, . . .	2 3, . . . 33, . . .	$\bar{1}'$ $\bar{3}', \ldots$ $3'', \ldots$ (in part)	∞''
Translation	T	—	—		$\mathbf{T}$
Gli-reflexion	G	21_111 21_11_11 $21_11_11_1$	21_111 21_11_11 $21_11_11_1$	$a=m'$ n d	
Gli-rotation	V_2 $V_3, \ldots$	221_11 221_11_1 $31_11, \ldots$	221_11 221_11_1 $31_11, \ldots$	2_1 $3_1, \ldots$	
Gli-roto-reflexion	G_2 $G_6^6, \ldots$	2221_1 $621_1, \ldots$	2221_1 $621_1, \ldots$	$2_1'=g'$ $3_1', \ldots$	

symmetry of a 3-D sphere, thus: $\infty/m\,\infty\,\infty''$, or $\infty'\,\infty'\,\infty''$. This has as subgroups all the irreducible 4-D point groups, including those isomorphous with 4-D space groups, enumerated by Coxeter (1934, p. 601). No doubt the (unlisted) reducible groups, which may be formed as a product of two or more groups of lower dimension, are also subgroups of $\infty'\,\infty'\,\infty''$. If other dimensional invariances are added, then such products are sufficient to describe the resulting symmetry; a symbol for this kind of symmetry is composed by bracketing those parts of the symbol that refer to one of the multiplying subgroups. For example, if the dimensional invariance is 2, 4, as in plane color groups, there is freedom within a 2-D plane, and also rotationally within the 2-D 'color plane' that is completely perpendicular in 4-D. The symmetry group is a product of the symmetry groups representing two planes, that is, $(\infty m)(\infty m)$. Di-rotation is present, as when you simultaneously rotate $\pi/2$ and change from red to green in Belov & Tarkhova's (1956, p. 10) group '$P4_1$', but is not essential to a description of the symmetry, that is $(\infty m)(\infty m)\infty''=(\infty m)(\infty m)$.

I would like to express appreciation for helpful discussion and criticism by Gabrielle Donnay, Z. V. Jizba, Jan Korringa, and Adolph Pabst.

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Acta Cryst. (1961). **14**, 1242

Anisotropic Structure Factor Calculations.*

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(*Received* 21 *July* 1960 *and in revised form* 12 *January* 1961)

A general form of the anisotropic structure factor which is suitable for evaluation in any space group is presented. A simple scheme for specifying the space group symmetry avoids the use of special 'patches'. The suggested form in the case of general and most special positions reduces to a form which permits substantial savings in the time required to form the function arguments and is well adapted to computation of structure factors and derivatives on high speed digital computers.

Structure factor for general position

As was demonstrated by Levy (1956), the β_{ij} in the expression for the anisotropic temperature factor,

$$\exp\left(-\sum_{i=1}^{3}\sum_{j=1}^{3}\beta_{ij}h_ih_j\right),$$

for symmetrically related positions, transform as do the quadratic products of atomic coordinates, while ignoring translational components.

* Contribution No. 904. Work was performed in the Ames Laboratory of the U.S. Atomic Energy Commission.