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Report of a Subcommittee on the Nomenclature of *n*-Dimensional Crystallography. II. Symbols for arithmetic crystal classes, Bravais classes and space groups[1]

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The Second Report of the Subcommittee on the Nomenclature of *n*-Dimensional Crystallography recommends specific symbols for *R*-irreducible groups in 4 and higher dimensions (*n*D), for centrings, for Bravais classes, for arithmetic crystal classes and for space groups (space-group types). The relation with higher-dimensional crystallographic groups used for the description of aperiodic crystals is briefly discussed. The *Introduction* discusses the general definitions used in the Report.

1. Introduction

Recommended symbols for symmetry operations, lattice systems, families and geometric crystal classes in 4D, 5D and 6D have been presented in Report I (Janssen, Birman *et al.*, 1999). Similar recommendations are given in this Report for the symbols of crystallographic elements in *n*D, in particular for Bravais classes, centrings, arithmetic crystal classes and space-group types. We abbreviate the term 'space-group type' to 'space group', unless there is a reason to do otherwise. Some material that belongs to the topics of the first Report but was left out there will also be dealt with, in particular the question of symbols for (*R*-)irreducible point groups.

In principle, the crystallographic groups, arithmetic and geometric crystal classes, and space groups, are available in dimensions 1–6 *via* the program *CARAT*, developed in Aachen by W. Plesken and collaborators. It can be obtained *via* their web site http://wwwb.math.rwth-aachen.de/carat/index.html. The notation and presentation given there is not easily adapted for crystallographic use, but all the information is present. According to that source the number of various classes in dimensions up to six is

Dimension:	1	2	3	4	5	6
Families	1	4	6	23	32	91
Bravais classes	1	5	14	64	189	841
Geometric classes	2	10	32	227	955	7104
Arithmetic classes	2	13	73	710	6079	85311
Space groups	2	17	219	4783	222018	28927922

The numbers of families and Bravais classes have been published in Plesken & Schulz (2000) and Opgenorth *et al.* (1998), respectively. The numbers increase rapidly with the dimension. A natural consequence is that the symbols have to be more and more complex. Also, it is clear that tables of these higher-dimensional groups are impossible. Fortunately, the number of higher-dimensional space groups needed for the description of aperiodic crystals is much lower. For example, there are only 370 non-isomorphic space groups of this type in 4D. As in 3D, where there are 11 enantiomorphic pairs of space groups, enantiomorphism occurs in higher dimensions as well. The number of enantiomorphic pairs, however, is not given in the table above.

A short review of the terminology used, and the definitions of the main notions, is presented first. Definitions may also be found in Vol. A of *International Tables for Crystallography* (Hahn, 2002), referred to hereafter as *ITA*. The concepts are clarified by examples in the third section. Nomenclature and symbols are discussed in §§4–8. Recommendations are given in

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§9. Evidently, the choice of a symbol is a compromise between information richness and conciseness. It is, for that reason, also a matter of taste. Sometimes alternatives will be given. The practice should make it clear what is the best choice.

Precise definitions are often rather dry. To be precise, a mathematical formulation is needed, but the notions have a crystallographic basis and can be described in a more heuristic way. Although we have avoided as much as possible a mathematical symbolism, the section on definitions will not be easy to digest for everybody. Therefore, we have chosen a two-track approach. In §2, a mathematical formulation is given and, in §3, the same notions are introduced in a more descriptive way, with examples. The reader could choose to skip §2 and go directly to §3. To make the correspondence clearer, we have inserted a number of cross references.

2. Definitions and symbols

A distance exists in a Euclidean space that is invariant under rigid-motion transformations. These form the Euclidean group $E(n)$ in the n-dimensional Euclidean space. A subgroup of $E(n)$ is the group of translations $T(n)$. If an origin is chosen, then the subgroup of $E(n)$ leaving this origin invariant is the orthogonal group in n dimensions, denoted by $O(n)$. The subgroup of $E(n)$ leaving an arbitrary point invariant is conjugate to $O(n)$. The elements of $E(n)$ are pairs $\{R|t\}$ of an orthogonal transformation R and a translation t. The product of two elements is given by

$$\{R_1|t_1\}\{R_2|t_2\} = \{R_1R_2|t_1 + R_1t_2\}.$$

This is the definition of a semi-direct product. Similarly, the affine group is the semi-direct product of the group of translations and the group of non-singular linear transformations.

Definition 1: Crystallographic space group. An n-dimensional crystallographic space group G is a subgroup of $E(n)$ such that its subgroup of translations is generated by n independent translations.

Comment: A space group does not have a fixed point. The translations belonging to the space group form a subgroup, called the (translation) lattice. The points obtained from the origin by the translation lattice is called the (point) lattice of the space group. The set of orthogonal transformations R for all elements $\{R|t\}$ in the space group leaves the origin fixed and forms a group of transformations that leaves the lattice of the space group invariant. This group is the point group associated with the space group.

There are other space-group types than crystallographic. An arbitrary subgroup of $E(n)$ that leaves no point invariant (it is fixed-point free) is called a space group and the crystallographic space groups are just special cases. In general, the translation subgroup is not generated by n independent translations. This is the case if the translation subgroup does not span the whole space, as for band and frieze groups. It also occurs if the translation subgroup is not generated by n independent translations but by more. For example, the translation group in 2D generated by five vectors making an angle of $2\pi/5$ with each other is generated by at least four translations. Then the generated point set becomes dense and the space group is not crystallographic. When there is no ambiguity, 'crystallographic space group' may be abbreviated to 'space group'.

Definition 2: Crystallographic point group. A subgroup of $O(n)$ is a crystallographic point group if it leaves an n-dimensional lattice invariant.

Comment: The translation subgroup of a space group G is an invariant subgroup and the factor group is isomorphic to the point group K. Moreover, the point group leaves the lattice invariant and is for that reason a crystallographic point group. A crystallographic point group is finite.

Definition 3: Geometric crystal class. Two point groups are called equivalent if they are conjugate subgroups of the orthogonal group $O(n)$. The equivalence classes for the crystallographic point groups are called the geometric crystal classes.

Definition 4: Equivalence of space groups. Two (crystallographic) space groups are called equivalent if they are conjugate subgroups of the affine group. By Bieberbach's theorem (Bieberbach, 1911), this is equivalent to stating that two crystallographic space groups are equivalent if they are isomorphic. The equivalence class of a space group is called the space-group type.

Definition 5: Holohedry. The holohedry of a lattice is the point group consisting of all orthogonal transformations leaving the lattice invariant.

Definition 6: Lattice system. Two lattices belong to the same lattice system if their holohedries are geometrically equivalent.

A lattice is spanned by n translation vectors $\mathbf{a}_1, \mathbf{a}_2, \ldots \mathbf{a}_n$. The lattice is then characterized by the scalar products.

Definition 7: Metric tensor. The metric tensor of a lattice is the tensor with elements $\mathbf{g}_{ij} = \mathbf{a}_i \cdot \mathbf{a}_j$.

Under an element of a point group K, the basis $\mathbf{a}_i$ transforms to a basis $\mathbf{b}_i$ and the metric tensor transforms to the tensor with elements

$$\mathbf{g}'_{ij} = \mathbf{b}_i \cdot \mathbf{b}_j = \sum_{kl} R_{ki}R_{lj}\mathbf{g}_{kl} \leftrightarrow \mathbf{g}' = R^{\mathrm{T}}\mathbf{g}R.$$

Here the superscript T denotes the transpose.

Because point groups are subgroups of $O(n)$, they can be presented as groups of orthogonal matrices, on an orthonormal basis. The group of all orthogonal matrices will also be denoted by $O(n)$. A crystallographic point group leaves an n-dimensional lattice invariant. Therefore, on a basis of such an invariant lattice, they are presented as groups of (invertible) integer matrices. The group of all n-dimensional invertible integer matrices is denoted by $\mathrm{GL}(n, \mathbb{Z})$.

Definition 8: Arithmetic point group. An arithmetic point group is a finite group of nD integer matrices.

Comment: The group of matrices presenting the nD crystallographic point group K depends on the choice of basis for the invariant lattice. Another basis is obtained from the first by an element of $\mathrm{GL}(n, \mathbb{Z})$. Therefore, the point group K corresponds to the set of all arithmetic groups that are conjugate in $GL(n, \mathbb{Z})$ to the first. This leads to a new equivalence.

Definition 9: Arithmetic crystal class. Two arithmetic point groups belong to the same arithmetic crystal class if they are conjugate subgroups of $GL(n, \mathbb{Z})$.

Two crystallographic point groups in the same geometric crystal class correspond after a choice of invariant lattice basis to two arithmetic point groups that are conjugate by a rational matrix. If there is a conjugating integer matrix, then the two groups are arithmetically equivalent, otherwise at least geometrically equivalent. This means that we can define the geometric crystal class of an arithmetic point group as the set of all arithmetic point groups conjugate to the first by a rational matrix. This implies that each geometric crystal class consists of complete arithmetic crystal classes. In other words, if two arithmetic point groups are arithmetically equivalent they are also geometrically equivalent.

The point group of a space group becomes an arithmetic point group on a basis that is a basis for the lattice of the space group. Any other lattice basis will lead to an arithmetically equivalent arithmetic group. Therefore, a space group determines an arithmetic crystal class, and consequently also a geometric crystal class. *Par abus de langage*, space groups may be considered to belong to a well determined arithmetic and geometric crystal class.

In the following, we shall make no distinction between point groups as groups of transformations or as groups of matrices. Because a space-group element is a pair of an orthogonal transformation and a translation, which correspond to an n-dimensional matrix and an n-dimensional vector, respectively, the space-group element may also be associated with a pair of an integer matrix and a (real) vector. This is sometimes conveniently presented as an $(n+1)$-dimensional matrix

$$\begin{pmatrix} R & t \\ 0 & 1 \end{pmatrix}.$$

Definition 10: Arithmetic holohedry. The arithmetic holohedry of a lattice with metric tensor g is the group of invertible integer matrices $D(R)$ such that $D(R)^{\mathrm{T}}\mathbf{g}D(R) = \mathbf{g}$.

Comment: Because the metric is left invariant, the group is equivalent to a group of orthogonal matrices. Because the group leaves the lattice invariant, it is a finite subgroup of $GL(n, \mathbb{Z})$.

Definition 11: Bravais class. Two lattices belong to the same Bravais class if their arithmetic holohedries are arithmetically equivalent.

Comment: Because two arithmetically equivalent (arithmetic) point groups are also geometrically equivalent, each lattice system consists of whole Bravais classes.

Definition 12: Bravais group. The set of tensors left invariant by an arithmetic point group $D(K)$ is denoted by S_K and defined as the set of metric tensors g for which

$$D(R)^{\mathrm{T}}\mathbf{g}D(R) = \mathbf{g}$$

for every R in K. Then the Bravais group of $D(K)$ is the group of all integer matrices $D(R)$ leaving all tensors in S_K invariant:

$$B(K) = \{D(R) \in GL(n, \mathbb{Z}) | D(R)^{\mathrm{T}}\mathbf{g}D(R) = \mathbf{g}, \text{ all } \mathbf{g} \text{ in } S_K\}.$$

Definition 13: Bravais class of an arithmetic point group. The Bravais group of an arithmetic point group is an arithmetic holohedry. Two arithmetic point groups belong to the same Bravais class if their Bravais groups are arithmetically equivalent.

In this way, arithmetic point groups (and therefore crystallographic space groups) may be grouped together. A coarser subdivision is given by the following.

Definition 14: Point-group system. Two geometric crystal classes belong to the same point-group system if there are two representatives of these classes with geometrically equivalent Bravais groups.

Definition 15: Family. A family of point groups (and of space groups) is the smallest union of point-group systems and Bravais classes of point groups such that with each crystallographic point group both its point-group system and its Bravais class belong to the union.

Comment: Since each space group determines an arithmetic crystal class and the Bravais class of its lattice, space groups and lattices can also be assigned to a well defined family.

Definition 16: Conventional lattice. In each family, one lattice is chosen such that the arithmetic holohedry of every lattice belonging to the family is equivalent by a rational matrix with the arithmetic holohedry of the chosen lattice, or one of its subgroups.

Comment: Usually, but not always, a lattice with a holohedry of maximal order is chosen. The rational matrix in the definition is the centring matrix. The determinant of its inverse is the number of points of the lattice inside the conventional unit cell. This number is called the *index* of the centred lattice in the conventional lattice. The arithmetic holohedry is usually chosen to show the reducibility of the holohedry, and to have the 'simplest' form. Especially the last criterion means that the choice is sometimes not unique. A basis for the conventional lattice is a *conventional basis*.

Definition 17: Reducibility. An arithmetic point group is $\mathbb{Z}$-reducible if there is an invariant sublattice of lower dimension. An arithmetic point group is R-reducible if there is a proper invariant subspace. An arithmetic point group is $\mathbb{Z}$- (or R-)irreducible if it is not $\mathbb{Z}$- (or R-)reducible.

Comment: One may distinguish between reducibility, decomposability and full reducibility. An arithmetic point group is $\mathbb{Z}$-reducible if by a basis transformation from $GL(n, \mathbb{Z})$ all elements may be brought to the form

$$\begin{pmatrix} A & B \\ 0 & D \end{pmatrix}$$

simultaneously, with the same dimensions of A, B and D for all elements. The group is $\mathbb{Z}$-decomposable if by such a basis transformation the elements may be brought into the form

$$\begin{pmatrix} A & 0 \\ 0 & D \end{pmatrix}$$

simultaneously. The group is fully reducible if the elements may be transformed by an element of $GL(n, \mathbb{Z})$ to a direct sum of ℤ-irreducible components. Similarly, the Q- and R-reducibility, Q- and R-decomposability and full Q- and R-reducibility are defined if the basis transformations are from GL(n, Q) and GL(n, R), respectively. ℤ-reducibility implies Q-reducibility, and the latter implies R-reducibility. On the other hand, R-irreducibility implies Q-irreducibility, and the latter implies ℤ-irreducibility.

Definition 18: Reducibility pattern of a crystallographic point group. The reducibility pattern is the space dimension n written as the sum of the dimensions of the irreducible components.

Comment: Generally, the reducibility pattern is different for the ℤ-reducibility and for the R-reducibility. The R-irreducible subspaces carry a real irreducible representation of the point group. The numbers in the reducibility pattern indicating the dimension of equivalent representations are enclosed in parentheses.

3. Explanation of the definitions

The definitions given above are somewhat mathematical in character, in order to be precise. Since their meanings, however, should be quite clear for crystallographers using them, some examples are now offered in which the definitions are discussed less formally.

Rigid motions in n dimensions (nD) are pairs of nD orthogonal transformations and nD translations. After the choice of an origin and a basis of the nD space, these rigid motions correspond to $n \times n$ matrices and nD vectors.

$$\left(\begin{pmatrix} R_{11} & \dots & R_{1n} \\ R_{21} & \dots & R_{2n} \\ \vdots & \ddots & \vdots \\ R_{n1} & \dots & R_{nn} \end{pmatrix} \middle| \begin{pmatrix} t_1 \\ t_2 \\ \vdots \\ t_n \end{pmatrix}\right).$$

An equivalent description, as used in *IT*A (Hahn, 2002), gives the transforms of an arbitrary point in the unit cell under the space-group elements, modulo the lattice translation vectors. For example, the groups $Pma2$ and $P2cm$ are given as follows.

$$\begin{array}{lllll} Pma2: & x,y,z & \bar{x},\bar{y},z & x+\frac{1}{2},\bar{y},z & \bar{x}+\frac{1}{2},y,z \\ P2cm: & x,y,z & x,\bar{y},\bar{z} & x,\bar{y},z+\frac{1}{2} & x,y,\bar{z}+\frac{1}{2}. \end{array}$$

This is a shorter way to give the transformation if there are many zeros in the matrix. A (crystallographic) space group is a group of rigid motions [**Definition 1**]. The corresponding orthogonal transformations form the point group [**Definition 2**], the translations form an nD lattice. On a basis of this lattice, the matrices of the point group have integer entries and are, generally, not orthogonal. By a change of basis S and of origin a, the matrices R and the vectors t change according to

$$R \to SRS^{-1}; \quad t \to St + (1 - SRS^{-1})a.$$

The 3D space groups $Pma2$ and $P2cm$ are equivalent *via* a basis transformation interchanging x and z.

Two space groups are considered to be identical if there is an origin shift and/or basis transformation that brings the matrices and translation vectors of the first into the same form as those of the second [**Definition 4**]. All space groups that are equivalent in this sense form an equivalence class. If there is a real basis transformation bringing the matrices of one point group in the same form as those of another, then the point groups belong to the same geometric crystal class [**Definition 3**]. A crystallographic point group with respect to an invariant lattice is a group of integer matrices. Two such groups are arithmetically equivalent if there is a basis transformation for one of the lattices such that the integer matrices become the same [**Definition 9**]. Because such lattice basis transformations are given by integer matrices, arithmetic equivalence is stronger than geometric equivalence. Geometric crystal classes contain complete arithmetic crystal classes. In 3D, there are 32 geometric crystal classes and 73 arithmetic crystal classes. The geometric crystal class $2/m$ contains two arithmetic crystal classes: $2/mP$ and $2/mC$.

The other definitions relate to the equivalence of lattices and the classification of space groups, and to the ordering of space and point groups in hierarchical structures. Lattices are characterized by the matrix of n^2 scalar products of the n basis vectors. This is the metric tensor [**Definition 7**]. For example, the metric tensor for a 3D monoclinic lattice is

$$\mathbf{g} = \begin{pmatrix} \mathbf{a}_1\cdot\mathbf{a}_1 & \mathbf{a}_1\cdot\mathbf{a}_2 & \mathbf{a}_1\cdot\mathbf{a}_3 \\ \mathbf{a}_1\cdot\mathbf{a}_2 & \mathbf{a}_2\cdot\mathbf{a}_2 & \mathbf{a}_2\cdot\mathbf{a}_3 \\ \mathbf{a}_1\cdot\mathbf{a}_3 & \mathbf{a}_2\cdot\mathbf{a}_3 & \mathbf{a}_3\cdot\mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} a & b & 0 \\ b & c & 0 \\ 0 & 0 & d \end{pmatrix}.$$

The subgroup of the orthogonal group that leaves the lattice invariant (each lattice point is transformed into a lattice point), the symmetry of the lattice, is the holohedry of the lattice [**Definition 5**]. For the lattice with metric tensor given above, the holohedry is just a point group of the geometric class $2/m$. Two lattices are considered to be equivalent if their symmetry groups are different settings of the same point group, which happens if the holohedries are in the same geometric crystal class. All lattices equivalent to a certain lattice form a lattice system [**Definition 6**]. All 3D cubic lattices (whether they are primitive, b.c.c. or f.c.c.) belong to one lattice system.

Because the holohedry leaves the lattice invariant, its matrices are integer if the chosen basis is a basis of the invariant lattice. As a group of integer matrices, it is called the arithmetic holohedry [**Definition 10**]. The adjective 'arithmetic' is used for groups of integer matrices and their crystal classes. The term 'arithmetic crystal class' is standard. Here we use the term arithmetic point group for any finite group of integer matrices [**Definition 8**] and arithmetic holohedry as well. Because a change of basis gives an arithmetic holohedry in the same arithmetic crystal class, one may introduce a finer classification of lattices. Two lattices are equivalent if their arithmetic holohedries are in the same arithmetic crystal class. The corresponding equivalence class of lattices is the Bravais class [**Definition 11**]. For example, there are 7 lattice systems but 14 Bravais classes in three dimensions.

For each arithmetic point group, there is a unique arithmetic holohedry as supergroup. It is called the Bravais group of the (arithmetic) point group [**Definition 12**]. The term

'Bravais' is used for the equivalence of lattices or for the holohedry of a lattice invariant under a given point group [**Definition 13**]. Every lattice left invariant under the 3D point group *mP* is also invariant under $2/mP$. At the same time, this is the largest group that leaves invariant all lattices invariant under *mP*. Therefore, $2/mP$ is the Bravais group of *mP*. It is the arithmetic holohedry of every primitive monoclinic lattice in 3D.

The lattice of a space group is invariant under its point group. Therefore, a choice of basis for the lattice gives a group of integer matrices, an arithmetic point group. A change of lattice basis gives an arithmetically equivalent group of matrices. Thus the space group determines a unique arithmetic crystal class. The classification hereafter branches, one branch going from arithmetic crystal classes to geometric crystal classes, and on to point-group systems, the other going from arithmetic crystal classes *via* Bravais groups to Bravais classes. Both branches come together in the most general classes: the families. (See Fig. 1 of Report I.)

As an example, the 3D space group $I4_1/a$ determines the arithmetic crystal class $4/mI$, which is contained in the geometric crystal class $4/m$. This belongs to the tetragonal system with holohedry $4/mmm$. On the other hand, the arithmetic point group $4/mI$ has $4/mmmI$ as its Bravais group. This is the arithmetic holohedry of the body-centred tetragonal Bravais class. In this case, the family has lattices with holohedry $4/mmm$. It is the tetragonal family.

The notions of system and family [**Definitions 14–15**] are exemplified by the case of the point groups in the hexagonal family in 3D. All lattices in this family have two free parameters. However, there are two systems, those with the rhombohedral lattice with holohedry $\bar{3}m$ and those with a hexagonal lattice with holohedry $6/mmm$.

The matrices of the point group on a lattice basis do not, in general, clearly show the character of the transformation. In many cases, this becomes clearer if a sublattice basis is chosen. The space-group lattice is obtained from the sublattice basis by the addition of vectors in the unit cell of the latter. This is the centring. The matrices and vectors corresponding to the orthogonal transformations and translations of the rigid motions then are given with respect to a conveniently chosen sublattice basis, the conventional basis [**Definition 16**].

In the 3D cubic family ($m\bar{3}m$), there are three Bravais classes: *P*, *I* and *F*. The reason for choosing *P* as the conventional lattice is to make the point-group matrices orthogonal, with each row and each column having precisely one non-zero entry. Both *I*- and *F*-lattices have a sublattice of the $m\bar{3}mP$ Bravais class. Bases for the two lattices are obtained from the conventional basis by (rational) basis transformations with determinant 1/2 and 1/4 (indices 2 and 4), respectively.

$$\tfrac{1}{2}\begin{pmatrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{pmatrix}; \quad \tfrac{1}{2}\begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}.$$

The centring may be given by the basis transformation or by the lattice vectors inside the conventional unit cell. For the examples, these are $0,0,0;\ \tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2}$ and $0,0,0;\ \tfrac{1}{2},\tfrac{1}{2},0;\ \tfrac{1}{2},0,\tfrac{1}{2};\ 0,\tfrac{1}{2},\tfrac{1}{2}$. The index of the *I*-lattice is two, that of the *F*-lattice is four.

Examples of the different types of (ir)reducibility [**Definition 17**] are the following. The group $2/mP$ in 3D with generating matrices

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

is $\mathbb{Z}$-reducible, $\mathbb{Z}$-decomposable and fully $\mathbb{Z}$-reducible (see the comments after Definition 17). Therefore, it is also fully *Q*- and *R*-reducible. The group *mc* in 2D with generating matrix

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

is $\mathbb{Z}$-reducible, but not $\mathbb{Z}$-decomposable. It is *Q*-decomposable and fully *Q*-reducible, and hence also fully *R*-reducible. The point group $[8]P_4$ in 4D generated by

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

is $\mathbb{Z}$- and *Q*-irreducible, but fully *R*-reducible. The cubic group $m\bar{3}mP$ is *R*-irreducible, and hence also *Q*- and $\mathbb{Z}$-irreducible.

Examples of the *R*-reducibility patterns [**Definition 18**] in 3D are the following:

Point group	Pattern	Comments
$\bar{1}$	(1+1+1)	*xyz* space for the single irrep.
$2/m$	(1+1)+1	*xy* plane for one irrep, the *z* axis for another.
mmm	1+1+1	three different one-dimensional representations.
$4/mmm$	2+1	invariant *xy* plane and invariant *z* axis.
$6/mmm$	2+1	invariant *xy* plane and invariant *z* axis.
$m\bar{3}m$	3	three-dimensional irrep.

In each symbol, the dimensions of the irreducible representations appearing in the point group are given, adding up to *n*. Equivalent irreducible components are put in parentheses.

The distinction between $\mathbb{Z}$- and *R*-reducibility patterns is illustrated with the following examples in 4D:

Point group	*R* pattern	$\mathbb{Z}$ pattern
$6m\perp6m$	2+2	2+2
$5m(5^2m)$	2+2	4
$m\bar{3}m.[8]$	4	4

The first point group may be brought into reduced form by integer matrices, and hence also by real matrices. The second only by a real matrix, the third not by a real matrix and hence neither by an integer matrix.

Table 1
Tables of R-irreducible geometric crystal classes in four dimensions.

(*a*) The geometric crystal classes of the four-dimensional family 21.

System	Order	Symbol	Alternative	BBNWZ No.
21_1	20	$[5].\bar{4}$		31/01
	40	$[5].\bar{4} \times \bar{1}_4$	$[10].\bar{4}$	31/02
	60	$[5].(23)$		31/03
	120	$[5].(23)\times\bar{1}_4$	$[10].(23)$	31/04
	120	$[5].(23).\bar{1}$	$[5].(\bar{4}.3.\bar{1})$	31/05
	120	$[5].(\bar{4}3m)$		31/06
	240	$[5].(\bar{4}3m)\times\bar{1}_4$	$[10].(\bar{4}3m)$	31/07

(*b*) The geometric crystal classes of the four-dimensional family 22.

System	Order	Symbol	Alternative	BBNWZ No.
22_1	18	$3\perp 3.2$	63.3	29/01
	36	$61(63).2$	66.63	29/02
	36	$3m1(1m3).2$	63.32	29/03
	36	$3m1(1m3).\bar{4}_{[36]}$	$\bar{4}.3\perp 3$	29/04
	72	$6m1(6m3).2$	$(66.63)\times\bar{1}_4$	29/05
	72	$6m1(6m3).\bar{4}_{[72]}$	$(\bar{4}.3\perp 3))\times\bar{1}_4$	29/06
	72	$3m\perp 3m.2$	$\bar{4}2m.(3\perp 3)$	29/07
	72	$6m1(m63).2_{[72]}$	$\bar{4}.\bar{3}.3$	29/08
	144	$6m11(613m).2$	$(63.2).\bar{3}m$	29/09
22_2	12	$6(6).\bar{4}_{[12]}$	44.33	30/01
	24	$6m(6m).44_{[24]}$	$(44\times 2).33$	30/02
	24	$61(32).44_{[24]}$	$[12].63_{[24]}$	30/03
	24	$6m(6m).2$	$(66.2).63_{[24]}$	30/04
	36	$61(63).44_{[36]}$	$[12].3$	30/05
	48	$6m1(3m2).44_{[48]}$	$[12].222$	30/06
	72	$6\perp 6.44_{[72]}$	$[12].6$	30/07
	72	$6m1(6m3).2$	$63.62.2$	30/08
	72	$6m1(6m3).44_{[72]}$	$[12].3.[12]_{[72]}$	30/09
	144	$6m1(1m6).2$	$[12].(622)$	30/10
	144	$6m1(1m6).\bar{4}_{[144]}$	$(6\perp 6).\bar{4}$	30/11
	144	$6m11(613m).44_{[144]}$	$[12].\bar{3}m$	30/12
	288	$6mm\perp 6mm.2$	$([12].2).6mm$	30/13

(*c*) The geometric crystal classes of the four-dimensional family 23.

System	Order	Symbol	Alternative	BBNWZ No.
23_1	8	44.44	$44.44_{[8]}$	32/01
	16	$[8].2.[8]$	$[8].[8]_{[16]}$	32/02
	16	$[8].44.2$	$[8].(44.2)_{[16]}$	32/03
	16	$44.44.2$	$44.(44\times 2)_{[16]}$	32/04
	24	$44.44.3$	62.44	32/05
	32	$[8].2.2$	$([8].2).44_{[32]}$	32/06
	32	$[8].[8].[8]$	$[8].[8].[8]_{[32]}$	32/07
	32	$[8].(4\perp 4)$	$[8].4$	32/08
	32	$44.\bar{4}.2$	$(44.2).\bar{4}$	32/09
	32	$44.44.(222)$	$(44\times 2).(44 \times 2)_{[32]}$	32/10
	48	$[8].44.3$	$[8].62$	32/11
	64	$\bar{4}.4\perp 4.\bar{4}$	$[8].(422)$	32/12
	64	$[8].\bar{4}.m$	$[8].mmm$	32/13
	64	$44.44.\bar{4}$	$(44.44).mmm_{[64]}$	32/14
	64	$(4\perp 4).\bar{4}$	$(4\perp 4).\bar{4}$	32/15
	96	$(23).44$	$(44\times 2).(23)$	32/16
	128	$[8].(4\perp 4).m$	$[8].(4\perp 4)$	32/17
	192	$(\bar{3}m).44$	$(44\times 2).m\bar{3}$	32/18
	192	$(\bar{4}3m).44$	$(44\times 2).\bar{4}3m$	32/19
	192	$(432).44$	$[8].432$	32/20
	384	$[8].m\bar{3}m$	$4.3.2.mmmm$	32/21
23_2	24	$[12].[12]_{[24]}$		33/01
	24	$[8].33$		33/02
	24	66.44		33/03
	48	$[12].[8]_{[48]}$		33/04
	48	$[12].(44\times 2)_{[48]}$		33/05
	48	$[8].66$		33/06
	72	$[12].62$		33/07
	96	$([12].[12]).222_{[96]}$		33/08
	96	$([12].2).[8]_{[96]}$		33/09
	96	$[12].(4\perp 2)$		33/10
	144	$([12].[8]).3_{[144]}$		33/11
	192	$[12].(4\perp 4)$		33/12
	288	$([12].[12]).23_{[288]}$		33/13
	576	$([12].[12]).\bar{4}3m_{[576]}$		33/14
	576	$([12].2).(432)$		33/15
	1152	$([12].2).m\bar{3}m$		33/16

4. Geometric crystal classes revisited

Symbols for R-reducible geometric classes were recommended in Report I, based on the symbols for geometric crystal classes in lower dimensions but not a notation for the R-irreducible cases. As the proposed symbols were generalizations of the Hermann–Mauguin symbols, it is logical to use this same approach for the R-irreducible classes. The Hermann–Mauguin symbols are based on the choice of a set of generators for a point group in the class. These generators are given by the corresponding symbols for orthogonal transformations, as presented for arbitrary dimensions in Report I.

The symbols should be unique, in the sense that a given symbol should correspond only to one geometric crystal class. Moreover, the symbol should give as much information about the structure of the group as is compatible with conciseness. The latter condition tends to smaller sets of generators. The mutual orientation of the symmetry operators, *i.e.* the mutual orientation of axes and invariant subspaces is clear for R-reducible point groups in 3D, but is not clear for R-irreducible cubic groups. The orientation of the mirror planes in the symbol $m\bar{3}m$, with respect to the threefold rotation axis, is not directly specified. This same problem occurs often in higher-dimensional spaces.

More information about a point group may be given by using the property that a point group may often be constructed as the product of some of its subgroups. The product may be indicated by '$\times$' when the product is a direct product or by a dot '.' for the general case. When the point group is the direct product of two subgroups acting in mutually perpendicular subspaces, the direct product is indicated by the symbol $\perp$. The Hermann–Mauguin symbol may be generalized by composing the symbol for the whole group from the symbols for these generating subgroups, some of which can be cyclic, in which case their symbol is just the symbol for a generator. A complicating factor now is that the symbols for orthogonal transformations often consist of more than one character. For example, the symbol 32 represents both a four-dimensional rotation (a threefold rotation in a two-dimensional subspace and a twofold rotation in a perpendicular two-dimensional subspace) and a three-dimensional point group of order six in the hexagonal family. It is important to clarify which of the two meanings the symbol represents when used for a higher-dimensional point group. We recommend placing the symbol for a point group in parentheses if it forms one of the generating point groups for the case under consideration, unless no confusion is possible. The symbol $3m$ only occurs for a 3D point group of order six,

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Table 2
Some R-irreducible point groups in 2–6 dimensions.

Dim.	Order	Generators	Symbol
2	12	$3,m,2$	$6mm$
3	48	$\bar{4},3,m$	$m\bar{3}m$
4	240	$m,3,\bar{4},[5]$	$[10].\bar{4}3m$
5	1440	$m,3,\bar{4},[5],\overline{63},\overline{1_5}$	$\overline{63}.\overline{[5]}.\bar{4}3m$
6	10080	$m,3,\bar{4},[5],\overline{63},[7],\overline{1_4}$	$\overline{[7]}.\overline{63}.[5].\bar{4}3m$
4	384	$\bar{4},3,2,m_x,m_y,m_z,m_u$	$4.3.2.mmmm$
5	3840	$[5],\bar{4},3,2,m_x,m_y,m_z,m_u,m_v$	$[5].4.3.2.mmmmm$
6	46080	$\overline{63},[5],\bar{4},3,2,m_x,m_y,m_z,m_u,m_v,m_w$	$63.[5].4.3.2.mmmmmm$

not as a symbol for an orthogonal transformation. In that case, parentheses are not necessary.

An example of a point group that requires parentheses is $(32)\times 44$ obtained by taking the direct product of the 3D point group 32 and the 4D cyclic group generated by an orthogonal transformation 44; 32×44 is the direct product of two cyclic groups, one with the sixfold rotation 32 as generator, the other with the fourfold rotation 44.

The order of the group is not necessarily the product of the orders of the generating subgroups. Although it is not always possible to choose subgroups generating the full group in such a way that the product of their orders is the order of the full group, it is convenient to make such a choice, whenever possible, because this immediately gives information about the group. In Table 1, recommendations are made for symbols of the R-irreducible point groups in four dimensions, belonging to the families 21–23 (Table 4 in Report I). This supplements Table 3 in Report I. For comparison, in addition to the recommended symbol the number in Brown *et al.* (1978) is given (BBNWZ No.). In Table 2, some examples of R-irreducible point groups are given in five and six dimensions.

There are several infinite series of R-irreducible groups with very similar structure in various dimensions. The use of similar symbols is recommended in these cases. The first series is that of hypercubic groups, generated by the permutations of the n axes and the n mirrors perpendicular to the axes. Their order is hence $2^n.n!$. The first members of the series are the 2D group $4mm$ and the 3D group $m\bar{3}m$. A second series is that of the symmetry groups of the generalized $(n+1)$D rhombohedral lattices, of order $2.(n+1)!$. The lattice is the projection of a generalized rhombohedral lattice on a hyperplane perpendicular to the diagonal of the unit cell. The first members are $6mm$ and $m\bar{3}m$. The third series is that of the symmetry groups of lattices that are the direct sum of a number of identical lower-dimensional lattices. An example is related to the group $6mm\perp 6mm$, the symmetry group of the sum of two 2D hexagonal lattices, of order 144. In case the two hexagonal lattices have the same lattice constant, there is a symmetry operation in 4D that exchanges the two lattices. The full symmetry group then is a group of order 288, with subgroup $6mm\perp 6mm$ of index two. Subgroups in this point-group system all have a subgroup of index 2 that is the subdirect product of two subgroups of $6mm$. This subgroup is (2+2)-reducible, and has been assigned a symbol in Report I. In addition, there is one additional generator, exchanging the two invariant subspaces.

The hypercubic lattice in 4D has the special property that there is a centred lattice for which the holohedry is of higher order than the hypercubic lattice. There is a threefold rotation permuting the 3 centring axes that belongs to the holohedry of the centred lattice but not to that of the hypercubic lattice. This threefold rotation is an additional generator which raises the order of the holohedry from 384 to 1152. Because the matrices of the group of order 384 on an orthonormal basis of the hypercubic lattice are simpler, the latter is chosen as the conventional lattice.

Proposals for the symbols of all R-irreducible geometric classes in 4D and for some in 5D and 6D are given in Tables 1 and 2. These are based on the considerations given above. For an alternative view, *cf.* Weigel *et al.* (2001) and, specifically for 5D, Veysseyre & Veysseyre (2002) and Veysseyre *et al.* (2002).

First example. The third group of system 21_1 in Table 1(a) has order 60. There are 12 group elements that, on the chosen basis, correspond to orthogonal matrices. These 12 form a subgroup, generated by

$$A=\begin{pmatrix}0&1&0&0\\0&0&0&1\\0&0&1&0\\1&0&0&0\end{pmatrix},\quad B=\begin{pmatrix}0&0&0&1\\0&0&1&0\\0&1&0&0\\1&0&0&0\end{pmatrix},$$

with relations $A^3=B^2=(AB)^3=E$. They form a 3D tetrahedral group 23 in the space perpendicular to the invariant vector $(1,1,1,1)$. In addition, the group has a generator

$$C=\begin{pmatrix}0&0&0&-1\\1&0&0&-1\\0&1&0&-1\\0&0&1&-1\end{pmatrix}.$$

This element generates a cyclic subgroup [5]. The two subgroups generate the full 4D point group with symbol [5].(23). Because the product of the orders of the two groups (5 and 12) is equal to the order of the group, the latter does not have to be given explicitly.

Second example. The second point group in the system 22_2 in Table 1(b) has order 24. There is an R-reducible subgroup generated by the matrices

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

of order 12. It is the group $6m(6m)$. In addition, there is a generator

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

The last matrix generates a cyclic group of order 4. It is the group 44. The symbol for the full group then is $6m(6m).44$ but,

Table 3
Centrings in 4D and their symbols.

Index	Matrix	Points in unit cell	BBNWZ	Recommended
2	$\frac{1}{2}\begin{pmatrix} 1 & 1 & 1 & 1 \\ -1 & 1 & 1 & 1 \\ 1 & -1 & 1 & 1 \\ 1 & 1 & -1 & 1 \end{pmatrix}$	$\begin{matrix} 0 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{matrix}$	*Z*	I_4
2	$\frac{1}{2}\begin{pmatrix} 1 & 1 & 1 & 0 \\ -1 & 1 & 1 & 0 \\ 1 & -1 & 1 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix}$	$\begin{matrix} 0 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & 0 \end{matrix}$	*I*	I_{xyz}
2	$\frac{1}{2}\begin{pmatrix} 1 & -1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix}$	$\begin{matrix} 0 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 \end{matrix}$	*S*(1,2)	I_{xy}
3	$\frac{1}{3}\begin{pmatrix} 2 & 1 & 1 & 0 \\ -1 & 1 & -1 & 0 \\ -1 & -2 & 1 & 0 \\ 0 & 0 & 0 & 3 \end{pmatrix}$	$\begin{matrix} 0 & 0 & 0 & 0 \\ \frac{2}{3} & \frac{1}{3} & \frac{1}{3} & 0 \\ \frac{1}{3} & \frac{2}{3} & \frac{2}{3} & 0 \end{matrix}$	*R*(1,2,3)	R_{xyz}
3	$\frac{1}{3}\begin{pmatrix} 1 & 1 & 1 & 1 \\ -2 & 1 & 1 & 1 \\ 1 & -2 & 1 & 1 \\ 1 & 1 & -2 & 1 \end{pmatrix}$	$\begin{matrix} 0 & 0 & 0 & 0 \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ \frac{2}{3} & \frac{2}{3} & \frac{2}{3} & \frac{2}{3} \end{matrix}$	RR_1	R_4
4	$\frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \\ 0 & -1 & 1 & 0 \\ -1 & 0 & 0 & 1 \end{pmatrix}$	$\begin{matrix} 0 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & \frac{1}{2} \\ 0 & \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{matrix}$	*D*(1,4)(2,3)	$I_{xu,yz}$
4	$\frac{1}{2}\begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix}$	$\begin{matrix} 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 \end{matrix}$	*F*(1,2,3)	F_{xyz}
4	$\frac{1}{2}\begin{pmatrix} 1 & -1 & 1 & 0 \\ 0 & 0 & -1 & 1 \\ 1 & 1 & 0 & -1 \\ 1 & 1 & 0 & 1 \end{pmatrix}$	$\begin{matrix} 0 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 0 & \frac{1}{2} & \frac{1}{2} \end{matrix}$	*G*(3,4)	$I_{xyz,zu}$
5	$\frac{1}{5}\begin{pmatrix} -1 & -1 & -1 & 4 \\ -1 & -1 & 4 & -1 \\ -1 & 4 & -1 & -1 \\ 4 & -1 & -1 & -1 \end{pmatrix}$	$\begin{matrix} 0 & 0 & 0 & 0 \\ \frac{1}{5} & \frac{1}{5} & \frac{1}{5} & \frac{1}{5} \\ \frac{2}{5} & \frac{2}{5} & \frac{2}{5} & \frac{2}{5} \\ \frac{3}{5} & \frac{3}{5} & \frac{3}{5} & \frac{3}{5} \\ \frac{4}{5} & \frac{4}{5} & \frac{4}{5} & \frac{4}{5} \end{matrix}$	*SN* inverse	Q_4
6	$\frac{1}{6}\begin{pmatrix} 2 & -2 & 1 & 3 \\ 2 & 4 & 1 & 3 \\ 0 & 0 & 3 & -3 \\ 0 & 0 & 3 & 3 \end{pmatrix}$	$\begin{matrix} 0 & 0 & 0 & 0 \\ \frac{1}{3} & \frac{2}{3} & \frac{1}{6} & \frac{1}{2} \\ \frac{2}{3} & \frac{1}{3} & \frac{1}{3} & 0 \\ 0 & 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{3} & \frac{2}{3} & \frac{2}{3} & 0 \\ \frac{2}{3} & \frac{1}{3} & \frac{5}{6} & \frac{1}{2} \end{matrix}$	*RS*(3,4)(1,2,3)	$R_{xyz}I_{zu}$
8	$\frac{1}{2}\begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 \\ -1 & -1 & -1 & 1 \end{pmatrix}$	$\begin{matrix} 0 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 \\ \frac{1}{2} & 0 & 0 & \frac{1}{2} \\ 0 & \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{matrix}$	*U*	F_4
8	$\frac{1}{4}\begin{pmatrix} 2 & 0 & 1 & 1 \\ 0 & 2 & 1 & -1 \\ 0 & -2 & 1 & -1 \\ -2 & 0 & 1 & 1 \end{pmatrix}$	$\begin{matrix} 0 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{2} & 0 & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{2} & 0 & \frac{3}{4} & \frac{3}{4} \\ 0 & \frac{1}{2} & \frac{3}{4} & \frac{1}{4} \\ 0 & \frac{1}{2} & \frac{1}{4} & \frac{3}{4} \end{matrix}$	*KG*(1,2)	$I_{xyz,zu}I_{xu}$

Table 3 (continued)

Index	Matrix	Points in unit cell	BBNWZ	Recommended
16	$\frac{1}{4}\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & -1 & 1 \\ -1 & 1 & -1 & 1 \\ -1 & -1 & 1 & 1 \end{pmatrix}$	$\begin{matrix} 0 & 0 & 0 & 0 \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{3}{4} & \frac{3}{4} & \frac{3}{4} & \frac{3}{4} \\ \frac{1}{4} & \frac{1}{4} & \frac{3}{4} & \frac{3}{4} \\ \frac{3}{4} & \frac{3}{4} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{3}{4} & \frac{1}{4} & \frac{3}{4} \\ \frac{3}{4} & \frac{1}{4} & \frac{3}{4} & \frac{1}{4} \\ \frac{3}{4} & \frac{1}{4} & \frac{1}{4} & \frac{3}{4} \\ \frac{1}{4} & \frac{3}{4} & \frac{3}{4} & \frac{1}{4} \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ 0 & 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 \\ 0 & \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{2} & 0 & 0 & \frac{1}{2} \\ 0 & \frac{1}{2} & \frac{1}{2} & 0 \end{matrix}$	KU	I_4F_4

because the product of the orders of the two subgroups is 48, the order of the group may be indicated explicitly: $6m(6m).44_{[24]}$.

5. Bravais classes and centrings

The symbol for a Bravais class is the symbol for the arithmetic holohedry of the Bravais class (de Wolff *et al.*, 1985, 1989, 1992). This consists of the symbol for the geometric class followed by a symbol for the centring, the latter being the basis transformation from a standard basis for the conventional cell to a primitive cell of a lattice from the Bravais class.

Centrings are given by the basis transformation from a conventional basis for the family to a primitive basis of the Bravais class. If the basis transformation is S, then the number of lattice translations in a unit cell of the conventional lattice is called the index of the centring, which is equal to the determinant of S. Conventionally, the basis transformation is given by a lower-case letter for 2D and an upper-case letter for 3D. We also recommend using one or more capital letters in higher dimensions.

The basis transformation can be specified either by the matrix S or by the lattice vectors inside a conventional unit cell. There are four cases that occur similarly for every dimension. One has index 1 and is indicated by P, another has index 2 and has, in addition to the origin, also the centre of the (conventional) unit cell; it is indicated by I. The third has three lattice translations along the diagonal of the unit cell and has symbol R, and the fourth has a lattice translation in the middle of each pair of conventional basis vectors. It has index 2^{n-1} in nD space and is indicated by F. If necessary to give the dimension explicitly, it may be added as a subindex: P_n, I_n, R_n and F_n. Centrings similar to R have m lattice translations along the diagonal and index m. We recommend that the centring be indicated by K for $m = 4$ and by Q for $m = 5$, or by K_n and Q_n, respectively.

Centrings of an mD sublattice, such as the C centring in a 3D orthorhombic lattice with centring translation $(0, 0, \frac{1}{2})$, are given by the same symbol as in lower dimensions but the centred sublattice must be indicated. We recommend using a subindex indicating the axes involved $(x, y, z, u, v, w, \ldots)$. Thus the C centring of the orthorhombic 3D lattice is given the symbol I_{xy}.

Finally, some centrings may be regarded as the centring of a centring. The basis transformation S is then given by the product of two basis transformations S_1 and S_2. The index of S is the product of the indices of S_1 and S_2. There is a centring with index 16 in 4D, for which the centring matrix can be viewed as the product of the centring matrix for I with that for F.

$$\frac{1}{2}\begin{pmatrix} 1 & 1 & 1 & 1 \\ -1 & 1 & 1 & 1 \\ 1 & -1 & 1 & 1 \\ 1 & 1 & -1 & 1 \end{pmatrix} \frac{1}{2}\begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 \\ -1 & -1 & -1 & 1 \end{pmatrix} = \frac{1}{4}\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & -1 & 1 \\ -1 & 1 & -1 & 1 \\ -1 & -1 & 1 & 1 \end{pmatrix}.$$

The symbol is then IF or I_4F_4. The basis vectors $[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$, $[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}, \frac{1}{4}]$, $[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$ and $[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$ span a lattice with 16 basis vectors in the conventional unit cell (see Table 3).

Products of sublattice centrings are treated in the same way. If the centrings have the same symbol, but possibly different orientations, then the subindices are combined. A centring in 4D with four lattice translations in the conventional unit cell given by $(0, 0, 0, 0)$, $(\frac{1}{2}, \frac{1}{2}, 0, 0)$, $(0, \frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ and $(\frac{1}{2}, 0, \frac{1}{2}, \frac{1}{2})$ is indicated by the centring symbol $I_{xy,yzu}$. This is, of course, the same as $I_{xy,xzu}$. As an example, all the centring symbols for 4D lattices are given in Table 3. Recommendations for the notation of the Bravais classes in 4D, using these centring symbols, are given in Table 4. Some examples of centring symbols for higher-dimensional (5D and 6D) spaces are given in Table 5.

Table 4
The 64 Bravais classes in 4D.

System	Holohedral point group	Centrings for Bravais classes
1_1	$\overline{1_4}$	P_4
2_1	$\bar{1}\perp m$	P_4, I_4
3_1	$2\perp 2$	P_4, I_4, $I_{xz,yu}$
4_1	$2\perp mm$	P_4, I_{zu}, I_{xyz}, I_4, $I_{xz,yu}$, F_{yzu}
5_1	4(4)	P_4
6_1	6(6)	P_4
7_1	$222\times\overline{1_4}$	F_4I_4
7_2	$mmmm$	P_4, I_{xy}, I_{xyz}, I_4, $I_{xy,uz}$, F_{xyz}, $I_{xyz,zu}$, F_4
8_1	$4mm\perp 2$	P_4, I_4
9_1	$\bar{3}m(m1)$	R_{xyz}
9_2	$6mm\perp 2$	P_4
10_1	$4m(4m)$	P_4, I_{xyz}, $I_{xu,yz}$
11_1	$6m(6m)$	P_4, R_4
12_1	$\bar{4}2m\times\overline{1_4}$	$I_{xyz,zu}I_{xu}$
12_2	$4mm\perp mm$	P_4, I_{zu}, I_{xyz}, I_4, $I_{xyz,zu}$
13_1	$\bar{3}m\perp m$	R_{xyz}, $R_{xyz}I_{zu}$
13_2	$6mm\perp mm$	P_4, I_{zu}
14_1	$8m(8^3m)$	P_4
15_1	$10m(10^3m)$	P_4
16_1	$12m(12^5m)$	P_4
17_1	$4m11(41mm)$	$I_{xu,yz}$
17_2	$4mm\perp 4mm$	P_4, I_4
18_1	$6mm\perp 4mm$	P_4
19_1	$m\bar{3}m(mm1)$	I_4F_4
19_2	$m\bar{3}m\perp m$	P_4, I_{xyz}, I_4, F_{xyz}, F_4
20_1	$6m1(3m2)$	$I_{yz,xyu}$
20_2	$6m11(613m)$	R_4
20_3	$6mm\perp 6mm$	P_4
21_1	$[10].\bar{4}3m$	P_4, Q_4
22_1	$6m11(613m).2$	R_4
22_2	$6mm\perp 6mm.2$	P_4
23_1	$[8].m\bar{3}m$	P_4
23_2	$[12].2.m\bar{3}m$	I_4

Table 5
Examples of centrings in 5D and 6D.

Symbol	Dimension	Index	Matrix
I_5	5	2	$\frac{1}{2}\begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ -1 & 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & 1 & 1 \\ 1 & 1 & -1 & 1 & 1 \\ 1 & 1 & 1 & -1 & 1 \end{pmatrix}$
I_6	6	2	$\frac{1}{2}\begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ -1 & 1 & 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & 1 & 1 & 1 \\ 1 & 1 & 1 & -1 & 1 & 1 \\ 1 & 1 & 1 & 1 & -1 & 1 \end{pmatrix}$
F_5	5	16	$\frac{1}{2}\begin{pmatrix} 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & -1 \end{pmatrix}$
F_6	6	32	$\frac{1}{2}\begin{pmatrix} 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$
I_{xy}	*e.g.* 4	2	$\frac{1}{2}\begin{pmatrix} 1 & -1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix}$
I_{xyzu}	*e.g.* 5	2	$\frac{1}{2}\begin{pmatrix} 1 & 1 & 1 & 1 & 0 \\ -1 & 1 & 1 & 1 & 0 \\ 1 & -1 & 1 & 1 & 0 \\ 1 & 1 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 2 \end{pmatrix}$
$I_{xy,zu,vw}$	*e.g.* 6	8	$\frac{1}{2}\begin{pmatrix} 1 & -1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & 0 & 1 & 1 \end{pmatrix}$

6. Arithmetic crystal classes

Two arithmetic point groups that are geometrically equivalent can be obtained from each other by a conjugation with a rational matrix. In other words, they are related by a centring matrix. As in the case for arithmetic crystal classes in one, two and three dimensions, the symbol for an arithmetic crystal class is the geometric crystal class symbol followed by a symbol for the centring of the lattice. However, a Bravais group may contain several subgroups that are geometrically equivalent but not arithmetically. A well known example in two dimensions is given by the pair of arithmetic groups $3m1p$ and $31mp$ of order 6. The difference between the two groups is the orientation of the mirror planes (m). In the first case, these are perpendicular to the crystal axes, in the second these are along the crystal axes. There are hence two ways to indicate point groups in the same geometric crystal class that are arithmetically different: either by the centring symbol or by indicating the orientation in the Bravais group.

Both approaches are used in 2D and 3D. In 3D, the point groups in the arithmetic crystal classes $3m1P$, $31mP$ and $3mR$ are geometrically equivalent. We recommend using the same system in higher dimensions, with the introduction of symbols for the centrings to distinguish between Bravais classes. The same symbols are used for the arithmetic crystal classes. In principle, there are more symbols than strictly needed for the Bravais classes. In 3D, the 14 Bravais classes would have the proposed general notation symbols $\bar{1}P_3$, $2/mP_3$, $2/mI_{xz}$, $mmmP_3$, $mmmI_3$, $mmmF_3$, $mmmI_{xy}$, $\bar{3}mR_3$, $6/mmmP_3$, $4/mmmP_3$, $4/mmmI_3$, $m\bar{3}mP_3$, $m\bar{3}mI_3$, $m\bar{3}mF_3$. Symbols such as I_{yz} are available for distinguishing between arithmetic crystal classes.

Different orientations of subgroups of the Bravais groups are indicated by the invariant spaces of the generators. This may be achieved by giving the axes in the invariant space of the element as superscripts.

A special case occurs if a generator of an R-reducible point group is the sum of mirrors in the various invariant subspaces. If the group is $\mathbb{Z}$-reducible with components of dimension less than 4, the orientation of the mirrors with respect to the crystal axes may be given. If the mirror plane is perpendicular to a crystal axis, the mirror is indicated by a dot ($\dot{m}$), otherwise by a double dot ($\ddot{m}$). This corresponds to the notation $m1$ and $1m$, respectively. The positional notation cannot be used here because combinations of a mirror of the first type in one subspace can be combined with one of the other type in another subspace. If the group is $\mathbb{Z}$-irreducible, but R-reducible, the same notation can be used with respect to the projection of the crystal axes on the invariant subspace. The case of twofold rotations instead of mirrors can be treated in the same way.

Example 1. The five arithmetic crystal classes in the geometric crystal class $m\bar{3}m\perp m$ are distinguished by the centrings. They are denoted as $m\bar{3}m\perp mP_4$, $m\bar{3}m\perp mI_4$, $m\bar{3}m\perp mI_{xyz}$, $m\bar{3}m\perp mF_{xyz}$ and $m\bar{3}m\perp mF_4$.

Example 2. In the geometric class $3m(3m)$, there are three arithmetic crystal classes. If the elements 33 and $2(=mm)$ are given by

$$A=\begin{pmatrix}0&-1&0&0\\1&-1&0&0\\0&0&0&-1\\0&0&1&-1\end{pmatrix},\quad B_1=\begin{pmatrix}-1&1&0&0\\0&1&0&0\\0&0&-1&1\\0&0&0&1\end{pmatrix},$$
$$B_2=\begin{pmatrix}1&-1&0&0\\0&-1&0&0\\0&0&1&-1\\0&0&0&-1\end{pmatrix},\quad B_3=\begin{pmatrix}-1&1&0&0\\0&1&0&0\\0&0&1&-1\\0&0&0&-1\end{pmatrix},$$

then three point groups, one from each class, are generated by A, B_1, or by A, B_2, or by A, B_3. The centring is primitive in all cases. Therefore, the symbols are, respectively, $3\dot{m}(3\dot{m})P_4$, $3\ddot{m}(3\ddot{m})P_4$, and $3\dot{m}(3\ddot{m})P_4$. Correspondingly, the two arithmetic classes in the geometric crystal class $6m(6m)$ are $6m(6m)P_4$ and $6\dot{m}(6\ddot{m})P_4$.

Example 3. The 4D geometric class $\bar{4}2m\times\bar{1}_4$ has 11 arithmetic classes. These correspond to the centrings P_4, I_4, I_{zu}, I_{xyu}, $I_{xyz,xyu}$ and N_4. For each of these centrings, except the last, there are two different orientations of the point group with respect to the crystal axes. One is generated by

$$A=\begin{pmatrix}0&1&0&0\\-1&0&0&0\\0&0&-1&0\\0&0&0&1\end{pmatrix},\quad B=\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&-1&0\\0&0&0&-1\end{pmatrix},$$
$$C=\begin{pmatrix}-1&0&0&0\\0&1&0&0\\0&0&-1&0\\0&0&0&1\end{pmatrix},$$

and the other by A, B and

$$D=\begin{pmatrix}0&1&0&0\\1&0&0&0\\0&0&-1&0\\0&0&0&1\end{pmatrix}.$$

The two arithmetic classes with P-centring are $\bar{4}2m\times\bar{1}_4P_4$ and $\bar{4}m2\times\bar{1}_4P_4$. The other arithmetic classes are similar, with other centrings, except the N-centring. In the latter case, only the second orientation occurs.

Table 6
Examples of arithmetic crystal classes in four dimensions.

(a) The arithmetic crystal classes of family $6mm\perp 2$.

Geometric class	Order	Arithmetic classes
3	3	$3P_4$, $3R_4$
$3m$	6	$3m1P_4$, $31mP_4$, $31mR_4$
$\bar{3}(m)$	6	$\bar{3}(m)P_4$, $\bar{3}(m)R_4$
$32(1m)$	6	$312(11m)P_4$, $312(11m)R_4$, $321(1m1)P_4$
$\bar{3}m(m1)$	12	$\bar{3}m1(m11)P_4$, $\bar{3}1m(m11)P_4$, $\bar{3}1m(m11)R_4$
6	6	$6P_4$
$3\perp 2$	6	$3\perp 2P_4$
$6mm$	12	$6mmP_4$
$6\perp 2$	12	$6\perp 2P_4$
$3m\perp 2$	12	$3m1\perp 2P_4$, $31m\perp 2P_4$
$6m(12)$	12	$6m(12)P_4$
$6mm\perp 2$	24	$6mm\perp 2P_4$

(b) The arithmetic crystal classes of family $mmmm$.

Geometric class	Order	Arithmetic classes
222	4	$222P_4$, $222I_4$, $222F_4$, $222I_4F_4$, $222I_{zu}$, $222I_{yz}$, $222I_{xyu}$, $222I_{xzu}$, $222I_{xz,yu}$, $222I_{xyz,zu}$, $222I_{xyu,yz}$, $222F_{xyz}$, $222F_{xyu}$
$222\times\overline{1_4}$	8	$222\times\overline{1_4}P_4$, $222\times\overline{1_4}I_4$, $222\times\overline{1_4}F_4$, $222\times\overline{1_4}I_4F_4$, $222\times\overline{1_4}I_{zu}$, $222\times\overline{1_4}I_{xyu}$, $222\times\overline{1_4}I_{xz,yu}$, $222\times\overline{1_4}I_{xyz,zu}$, $222\times\overline{1_4}F_{xyz}$
mmm	8	$mmmP_4$, $mmmI_4$, $mmmF_4$, $mmmI_{zu}$, $mmmI_{yz}$, $mmmI_{xyu}$, $mmmI_{xzu}$, $mmmI_{xz,yu}$, $mmmI_{xyz,zu}$, $mmmI_{xyu,yz}$, $mmmF_{xyz}$, $mmmF_{xyu}$
$222\perp m$	8	$222\perp mP_4$, $222\perp mI_4$, $222\perp mF_4$, $222\perp mI_{zu}$, $222\perp mI_{yu}$, $222\perp mI_{xyu}$, $222\perp mI_{xyz}$, $222\perp mI_{xz,yu}$ $222\perp mI_{xyz,zu}$, $222\perp mI_{xyz,yu}$, $222\perp mF_{xyz}$, $222\perp mI_{xzu}$
$mmmm$	16	$mmmmP_4$, $mmmmI_4$, $mmmmF_4$, $mmmmI_{zu}$, $mmmmI_{xyu}$, $mmmmI_{xz,yu}$, $mmmmI_{xyz,zu}$, $mmmmF_{xyz}$

Example 4. The geometric crystal class $[5].2 = 5m(5^2m)$ contains two arithmetic classes. A representative is generated by

$$A=\begin{pmatrix}0&0&0&-1\\1&0&0&-1\\0&1&0&-1\\0&0&1&-1\end{pmatrix},\quad B=\begin{pmatrix}0&0&0&1\\0&0&1&0\\0&1&0&0\\1&0&0&0\end{pmatrix},$$

and another by A and $C=-B$. The groups are $\mathbb{Z}$-irreducible, but R-reducible, and arithmetically non-equivalent. B and C are composed of two mirrors, one in each R-irreducible subspace. The mirrors in both subspaces go either through the projection of basis vectors of the lattice basis or they are both perpendicular. Therefore, the two arithmetic groups can be given the symbols $51m(5^21m)$ and $5m1(5^2m1)$, or $5\dot{m}(5^2\dot{m})$ and $5\ddot{m}(5^2\ddot{m})$.

Example 5. All arithmetic crystal classes for the two 4D families $6mm\perp 2$ and $mmmm$ are given in Table 6 with their recommended symbols.

Table 7
Examples of 4D space groups.

Arithmetic crystal class	Symbol	Generators
$[8].2.2P$	$P[8].2.2$	$(z, u, -y, x), (x, y, -z, -u), (x, -y, u, z)$
	$P[8].2.2_x$	$(z, u, -y, x+\frac{1}{2}), (x, y, -z+\frac{1}{2}, -u+\frac{1}{2}), (x+\frac{1}{2}, -y, u, z)$
	$P[8].2_{xy}.2$	$(z, u, -y, x), (x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{1}{2}, -u+\frac{1}{2}), (x, -y, u, z)$
$[8].2P$	$P[8].2$	$(-u, x, y, z), (-x, u, z, y)$
	$P[8].2_z$	$(-u, x, y, z+\frac{1}{2}), (-x, u, z+\frac{1}{2}, y)$
$4m\perp 2P$	$P4m\perp 2$	$(-y, x, z, u), (-x, y, z, u), (x, y, -z, -u)$
	$P4_{2u}m_{yu}\perp 2_{xy}$	$(-y+\frac{1}{2}, x, z, u+\frac{1}{2}), (-x, y+\frac{1}{2}, z, u+\frac{1}{2}), (x+\frac{1}{2}, y+\frac{1}{2}, -z, -u)$
	$P4_z m_{yu}\perp 2_{xy}$	$(-y+\frac{1}{2}, x, z+\frac{1}{2}, u), (-x, y+\frac{1}{2}, z, u+\frac{1}{2}), (x+\frac{1}{2}, y+\frac{1}{2}, -z, -u)$
	$P4m\perp 2_{xy}$	$(-y, x, z, u), (-x, y, z, u), (x+\frac{1}{2}, y+\frac{1}{2}, -z, -u)$
	$P4m_y\perp 2$	$(-y+\frac{1}{2}, x, z, u), (-x, y+\frac{1}{2}, z, u), (x, y, -z, -u)$
	$P4_{2u}m\perp 2$	$(-y, x, z, u+\frac{1}{2}), (-x, y, z, u), (x, y, -z, -u)$
	$P4m_y\perp 2_{xy}$	$(-y+\frac{1}{2}, x, z, u), (-x, y+\frac{1}{2}, z, u), (x+\frac{1}{2}, y+\frac{1}{2}, -z, -u)$
	$P4_{2u}m\perp 2_{xy}$	$(-y, x, z, u+\frac{1}{2}), (-x, y, z, u), (x+\frac{1}{2}, y+\frac{1}{2}, -z, -u)$
	$P4_{2u}m_z\perp 2_{xy}$	$(-y, x, z, u+\frac{1}{2}), (-x, y, z+\frac{1}{2}, u), (x+\frac{1}{2}, y+\frac{1}{2}, -z, -u)$
	$P4m_u\perp 2$	$(-y, x, z, u), (-x, y, z, u+\frac{1}{2}), (x, y, -z, -u)$
	$P4_{2u}m_y\perp 2$	$(-y+\frac{1}{2}, x, z, u+\frac{1}{2}), (-x, y+\frac{1}{2}, z, u), (x, y, -z, -u)$
	$P4_{2u}m_u\perp 2$	$(-y, x, z, u+\frac{1}{2}), (-x, y, z, u+\frac{1}{2}), (x, y, -z, -u)$
	$P4m_u\perp 2_{xy}$	$(-y, x, z, u), (-x, y, z, u+\frac{1}{2}), (x+\frac{1}{2}, y+\frac{1}{2}, -z, -u)$
	$P4_{2u}m_y\perp 2_{xy}$	$(-y+\frac{1}{2}, x, z, u+\frac{1}{2}), (-x, y+\frac{1}{2}, z, u), (x+\frac{1}{2}, y+\frac{1}{2}, -z, -u)$
	$P4_{2u}m_u\perp 2_{xy}$	$(-y, x, z, u+\frac{1}{2}), (-x, y, z, u+\frac{1}{2}), (x+\frac{1}{2}, y+\frac{1}{2}, -z, -u)$
	$P4_{2u}m_{yz}\perp 2$	$(-y+\frac{1}{2}, x, z, u+\frac{1}{2}), (-x, y+\frac{1}{2}, z+\frac{1}{2}, u), (x, y, -z, -u)$
	$P4m_{yu}\perp 2$	$(-y+\frac{1}{2}, x, z, u), (-x, y+\frac{1}{2}, z, u+\frac{1}{2}), (x, y, -z, -u)$
	$P4_{2u}m_{yu}\perp 2$	$(-y+\frac{1}{2}, x, z, u+\frac{1}{2}), (-x, y+\frac{1}{2}, z, u+\frac{1}{2}), (x, y, -z, -u)$
	$P4m_{yu}\perp 2_{xy}$	$(-y+\frac{1}{2}, x, z, u), (-x, y+\frac{1}{2}, z, u+\frac{1}{2}), (x+\frac{1}{2}, y+\frac{1}{2}, -z, -u)$
	$P4_{2u}m_z\perp 2$	$(-y, x, z, u+\frac{1}{2}), (-x, y, z+\frac{1}{2}, u), (x, y, -z, -u)$

7. Space groups

Space-group symbols are conveniently chosen as the symbols for the arithmetic crystal class corresponding to the space group, with additional information on the translation parts of the space-group elements. The intrinsic part of the corresponding translation in the space-group element is given in the symbol for every generator of the point group. This is the translation component that is invariant under origin shifts. In the symbols used up to the 3D case, a subindex represents the intrinsic part of the translation for a screw axis (*e.g.* $P2_1$), and for a glide reflection (*e.g.* $P2/a$) the mirror symbol 'm' is replaced by a letter that corresponds to the translation. With the de Wolff *et al.* (1992) nomenclature, the centring symbol for the arithmetic crystal class is placed at the beginning of the space-group symbol.

The same scheme can be adopted in higher dimensions. Each character in the symbol for a point group stands for a generator of the point group or a component of a generator. The latter occurs if an orthogonal transformation is indicated by more than one digit, as *e.g.* the 4D rotation 43 of order 12, or the element 6(6) in a 4D reducible point group. The intrinsic translations only appear in invariant subspaces. Therefore, the examples given [43 and 6(6)] hence have intrinsic translations only in spaces of dimension higher than 4. We recommend appending an index to the symbol to indicate the intrinsic translation. The position of the index is:

– for series of subsequent characters indicating an orthogonal transformation (such as 3 or 43), directly after the last character;

– for characters separated by parentheses, directly after the last character of the corresponding component, followed by an eventual component in other directions.

The intrinsic translation of a space-group element is always a rational fraction of a lattice translation in the invariant subspace. It can be given by that fraction and the lattice translation. Suppose the fraction is p/q and the order of the orthogonal transformation is n. Then np/q corresponds to a lattice translation. We take the order of the element (n) as the denominator. With respect to a primitive basis, np/q would be an integer, but, because translations are given with respect to the conventional basis, np/q still may be a fraction. This fraction is placed before the lattice translation vector indicated by $x\mathbf{e}_1 + y\mathbf{e}_2 + z\mathbf{e}_3 + \ldots$, where $\mathbf{e}_i$ is the ith basis vector.

It is sufficient to indicate the translation part for a set of generators because the other space-group elements including their translation parts are the result of multiplications. However, the intrinsic parts are not always sufficient. There are non-symmorphic space groups for which a set of generators may be chosen without an intrinsic translation part. An example is the 3D group $I2_12_12_1$. For every element of the point group, the associated translation in the space-group element may be changed by adding a lattice translation or by a change of origin. In the case of $I2_12_12_1$, there is an origin for which the rotation along the z axis has a translation $(\frac{1}{2}0\frac{1}{2})$ and the space-group element is a screw rotation. However, because $(\frac{1}{2}\frac{1}{2}\frac{1}{2})$ is a lattice translation, the translation in the screw rotation may be changed to $(0\frac{1}{2}0)$, which may be changed to zero by an origin shift. This holds for all three twofold rotations. However, the non-primitive translations cannot simultaneously be eliminated. The choice of generators of the point group without intrinsic translations would lead to the symbol $I222$, which is already the symbol for the symmorphic group. Therefore, the symbol $I2_12_12_1$ is used. We recommend choosing in similar situations translation components for which the intrinsic part is non-zero.

A similar situation occurs for the group $P5\bar{3}m(5^2\bar{3}m)$. Strictly speaking, the elements $5(5^2) = [5]$ and $\bar{3}(\bar{3}) = 662$ generate the point group. However, this choice leads to a notational problem. There is a non-symmorphic space group with generators $\{[5]|(0\frac{1}{2}\frac{1}{2}000)\}$ and $\{\bar{3}(\bar{3})|(00\frac{1}{2}0\frac{1}{2}0)\}$. Both translation parts may be eliminated by an origin shift. However, their product $m(m)$ has a translation part $(00\frac{1}{2}\frac{1}{2}00)$, which is intrinsic. Therefore, it is advisable to use the symbol $P5\bar{3}m_{zu}(5^2\bar{3}m)$. The non-symmorphic character can only be made evident by choosing $m(m)$ = 2 as a (superfluous) generator of the point group. We recommend using more generators for the point group than strictly necessary, if that is

Table 8
Space groups in five dimensions: system $10m(10^3m)\perp m$.

Generating matrices for the 5D groups below:

$$A = \begin{pmatrix} 0&1&0&0&0\\ 0&0&1&0&0\\ 0&0&0&1&0\\ 0&0&0&0&1\\ 1&0&0&0&0 \end{pmatrix},\quad B = \begin{pmatrix} 1&0&0&0&0\\ 0&0&0&0&1\\ 0&0&0&1&0\\ 0&0&1&0&0\\ 0&1&0&0&0 \end{pmatrix},\quad F = \begin{pmatrix} 1&0&0&0&0\\ 0&1&0&0&0\\ 0&0&1&0&0\\ 0&0&0&1&0\\ 0&0&0&0&-1 \end{pmatrix},\quad C = \begin{pmatrix} 0&1&-1&0&0\\ 0&1&0&-1&0\\ 0&1&0&0&0\\ -1&1&0&0&0\\ 0&0&0&0&1 \end{pmatrix},$$

$$D = \begin{pmatrix} 0&0&0&1&0\\ 0&0&1&0&0\\ 0&1&0&0&0\\ 1&0&0&0&0\\ 0&0&0&0&1 \end{pmatrix},\quad G = \begin{pmatrix} -1&0&0&0&0\\ -1&0&0&1&0\\ -1&0&1&0&0\\ -1&1&0&0&0\\ 0&0&0&0&1 \end{pmatrix},\quad A' = \begin{pmatrix} -1&-1&-1&-1&0\\ 1&0&0&0&0\\ 0&1&0&0&0\\ 0&0&1&0&0\\ 0&0&0&0&1 \end{pmatrix}\quad I \text{ is } \overline{1_5}.$$

(*a*) Examples of space groups in the five- and tenfold system in 5D: *Q*-centring.

Arithmetic crystal class	Generators	Translations	Space-group symbol	Alternative
$5(5^2)Q$	A	00000	$Q5(5^2)$	$Q5(5^2)$
$5m(5^2m)Q$	A, B	00000 00000	$Q5m(5^2m)$	$Q5m(5^2m)$
		00000 0000$\frac{1}{2}$	$Q5m_v(5^2m)$	$Q5c(5^2m)$
$5m(5^2m)(1m)Q$	$A, -B$	00000 00000	$Q5m(5^2m)\ (1m)$	$Q52(5^2m)$
$10(10^3)(m)Q$	$-A$	00000	$Q10(10^3)(m)$	$Q\bar{5}(10^3)$
$10m(10^3m)(m)Q$	$-A, B$	00000 00000	$Q10m(10^3m)(m)$	$Q\bar{5}m(10^3m)$
		00000 0000$\frac{1}{2}$	$Q10m_v(10^3m)(m)$	$Q\bar{5}c(10^3m)$

(*b*) Examples of space groups in the five- and tenfold system in 5D: *P*-centring.

Arithmetic crystal class	Generators	Translations	Space-group symbol	Alternative
$5(5^2)P$	A'	00000	$P5(5^2)$	$P5(5^2)$
		0000$\frac{1}{5}$	$P5_v(5^2)$	$P5_1(5^2)$
$5m(5^2m)P$	A', D	00000 00000	$P5m(5^2m)$	$P5m1(5^2m1)$
		00000 0000$\frac{1}{2}$	$P5m_v(5^2m)$	$P5c1(5^2m1)$
$5\dot{m}(5^2m)P$	A', G	00000 00000	$P5\dot{m}(5^2m)$	$P51m(5^21m)$
		00000 0000$\frac{1}{2}$	$P5\dot{m}_v(5^2m)$	$P51c(5^21m)$
$5m(5^2m)(1m)P$	$A', -D$	00000 00000	$P5m(5^2m)(1m)$	$P521(5^2m1)$
		0000$\frac{1}{5}$ 00000	$P5_vm(5^2m)(1m)$	$P5_121(5^2m1)$
$5\dot{m}(5^2m)(1m)P$	$A', -G$	00000 00000	$P5\dot{m}(5^2m)(1m)$	$P512(5^21m)$
		0000$\frac{1}{5}$ 00000	$P5_v\dot{m}(5^2m)(1m)$	$P5_112(5^21m)$
$10(10^3)(m)P$	$-A'$	00000	$P10(10^3)(m)$	$P\bar{5}(10^3)$
$10m(10^3m)(m1)P$	$-A', D$	00000 00000	$P10m(10^3m)(m1)$	$P\bar{5}m1(10^3m1)$
		00000 0000$\frac{1}{2}$	$P10m_v(10^3m)(m1)$	$P\bar{5}c1(10^3m1)$
$10\dot{m}(10^3m)(m1)P$	$-A', D$	00000 00000	$P10\dot{m}(10^3m)(m1)$	$P\bar{5}21(10^3m1)$
		00000 0000$\frac{1}{2}$	$P10\dot{m}_v(10^3m)(m1)$	$P\bar{5}2_11(10^3m1)$
$10(10^3)P$	C	00000	$P10(10^3)$	$P10(10^3)$
		0000$\frac{1}{10}$	$P10_v(10^3)$	$P10_1(10^3)$
		0000$\frac{1}{5}$	$P10_{2v}(10^3)$	$P10_2(10^3)$
		0000$\frac{1}{2}$	$P10_{5v}(10^3)$	$P10_5(10^3)$
$5(5^2)(m)P$	$-C$	00000	$P5(5^2)(m)$	$P\overline{10}(5^2)$
$10(10^3)\perp m$	C, F	00000 00000	$P10(10^3)\perp m$	$P10/m(10^3)$
		0000$\frac{1}{2}$ 00000	$P10_{5v}(10^3)\perp m$	$P10_5/m(10^3)$
$10m(10^3m)P$	C, D	00000 00000	$P10m(10^3m)$	$P10mm(10^3mm)$
		00000 0000$\frac{1}{2}$	$P10m_v(10^3m)$	$P10cc(10^3mm)$
		0000$\frac{1}{2}$ 00000	$P10_{5v}m(10^3m)$	$P10_5mc(10^3mm)$
		0000$\frac{1}{2}$ 0000$\frac{1}{2}$	$P10_{5v}m_v(10^3m)$	$P10_5cm(10^3mm)$
$10m(10^3m)(m)P$	$C, -B$	00000 00000	$P10m(10^3m)(m)$	$P10\ 22(10^3mm)$
		0000$\frac{1}{10}$ 00000	$P10_vm(10^3m)(m)$	$P10_122(10^3mm)$
		0000$\frac{1}{5}$ 00000	$P10_{2v}m(10^3m)(m)$	$P10_222(10^3mm)$
		0000$\frac{1}{2}$ 00000	$P10_{5e}m(10^3m)(m)$	$P10_522(10^3mm)$
$5m(5^2m)(m1)P$	$-C, B$	00000 00000	$P5m(5^2m)(m1)$	$P\overline{10}m1(5^2m1)$
		0000$\frac{1}{2}$ 00000	$P5_vm(5^2m)(m1)$	$P\overline{10}c1(5^2m1)$
$5\dot{m}(5^2m)(m1)P$	$-C, B$	00000 00000	$P5\dot{m}(5^2m)(m1)$	$P\overline{10}\ 1m(5^21m)$
		0000$\frac{1}{2}$ 00000	$P5_v\dot{m}(5^2m)(m1)$	$P\overline{10}\ 1c(5^21m)$
$10m(10^3m)\perp mP$	C, D, I	00000 00000 00000	$P10m(10^3m)\perp m$	$P10/mmm(10^31mm)$
		0000$\frac{1}{2}$ 0000 00000	$P10_{5v}m(10^3m)\perp m$	$P10_5/mmc(10^31mm)$
		00000 0000$\frac{1}{2}$ 00000	$P10m_v(10^3m)\perp m$	$P10/mcm(10^31mm)$
		0000$\frac{1}{2}$ 0000$\frac{1}{2}$ 00000	$P10_vm_v(10^3m)\perp m$	$P10_5/mcm(10^31mm)$

Table 9
Space groups in six dimensions; space groups for the arithmetic class $m\bar{3}m(m\bar{3}m)P_6$.

Generators	Symbol	Alternative
$(-y, x, z, -v, u, w)$ $(-y, -z, -x, -v, -w, -u)$	$Pm\bar{3}m(m\bar{3}m)$	$P4(4).662.2$
$(-y, x+\frac{1}{2}, z+\frac{1}{2}, -v+\frac{1}{2}, u, w)$ $(-y, -z, -x, -v, -w, -u)$	$Pn\bar{3}n(n\bar{3}n)$	$P4_z(4_w).662.2$
$(-y, x, z, -v+\frac{1}{2}, u, w)$ $(-y, -z, -x, -v, -w, -u)$	$Pm\bar{3}m(n\bar{3}n)$	$P4(4_w).662.2$
$(-y, x, z, -v, u+\frac{1}{2}, w+\frac{1}{2})$ $(-y, -z, -x, -v, -w, -u)$	$Pm\bar{3}m(n\bar{3}m)$	$P4(4).662.2_u$
$(-y, x, z, -v+\frac{1}{2}, u+\frac{1}{2}, w+\frac{1}{2})$ $(-y, -z, -x, -v, -w, -u)$	$Pm\bar{3}m(m\bar{3}n)$	$P4(4_w).662.2_u$

a way to indicate the character of the non-symmorphic space group.

1: The space group with generators

$$\left(\begin{pmatrix}-1&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&1\end{pmatrix}\middle|\begin{pmatrix}0\\0\\\frac{1}{2}\\0\end{pmatrix}\right),\quad \left(\begin{pmatrix}1&0&0&0\\0&-1&0&0\\0&0&1&0\\0&0&0&1\end{pmatrix}\middle|\begin{pmatrix}0\\0\\0\\\frac{1}{2}\end{pmatrix}\right),$$
$$\left(\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&-1&0\\0&0&0&-1\end{pmatrix}\middle|\begin{pmatrix}\frac{1}{2}\\\frac{1}{2}\\0\\0\end{pmatrix}\right)$$

(and the lattice translations) has arithmetic point group $mm\perp 2P$ and symbol $Pm_zm_u\perp 2_{xy}$.

2. The space group with the lattice translations and

$$\left(\begin{pmatrix}0&-1&0&0&0\\1&0&0&0&0\\0&0&0&-1&0\\0&0&1&0&0\\0&0&0&0&1\end{pmatrix}\middle|\begin{pmatrix}0\\0\\0\\0\\\frac{1}{2}\end{pmatrix}\right),$$
$$\left(\begin{pmatrix}-1&0&0&0&0\\0&1&0&0&0\\0&0&-1&0&0\\0&0&0&1&0\\0&0&0&0&1\end{pmatrix}\middle|\begin{pmatrix}0\\0\\0\\0\\\frac{1}{2}\end{pmatrix}\right).$$

as generators has arithmetic point group $4m(4m)P$. Because the order of the first rotation is four, the fraction $np/q = 2$ and four times the translation part is $2\mathbf{e}_5$. Although the translation part of the second generator is the same, the order of the second rotation is two and $np/q = 1$. Therefore, the symbol is $P4_{2v}m_v(4m)$.

Lists of space groups may be found in Brown *et al.* (1978) for 4D (a complete list), in Martinais (1987) for 6D and in Janssen (1988) for 5D and 6D.

This is not the place to give full lists of the recommended symbols for all space groups in dimensions higher than three. As examples, all space groups are given for a selected number of arithmetic crystal classes in 4D (Table 7), 5D (Table 8) and 6D (Tables 9 and 10). Generators for the space groups are given either by generating matrices for the arithmetic point group together with the associated translations (Table 8) or by the action of the generators on a point (x, y, z, u, v) in 5D or (x, y, z, u, v, w) in 6D (Tables 7, 9 and 10). For example, one generator of the space group $P5_x32(5^232)$ can be written as

$$(x+\tfrac{1}{5}, z, u+\tfrac{1}{5}, v, w, y-\tfrac{1}{5})$$

or as $A, \frac{1}{5}0\frac{1}{5}00-\frac{1}{5}$ with

$$A=\begin{pmatrix}1&0&0&0&0&0\\0&0&1&0&0&0\\0&0&0&1&0&0\\0&0&0&0&1&0\\0&0&0&0&0&1\\0&1&0&0&0&0\end{pmatrix}.$$

8. Symmetries of aperiodic crystals

Higher-dimensional crystallographic symmetry groups have been adopted in specifying the symmetry of quasiperiodic crystals, *i.e.* the aperiodic crystals for which the diffraction spots can be labelled by a finite set of integer indices. There are at least three different, but partly overlapping, classes among these aperiodic crystals: the incommensurate displacively/occupationally modulated phases, the incommensurate composites and the quasicrystals.

The symmetry groups of these structures are (3+d)-dimensional space groups, called superspace groups. These are space groups in a space that is the sum of the 3D physical space and a dD internal or perpendicular space. The dimension d is determined by the number $n = 3 + d$ of basis vectors of the Fourier module of the structure. This is the set of reciprocal-lattice vectors spanned with integer coefficients by the positions of the diffraction spots of the aperiodic crystal.

The point groups of these superspace groups are R-reducible in 3D and dD components, both possibly R-reducible themselves. Affine conjugation or isomorphism may be used as coarsest equivalence relation of superspace groups. For modulated structures, this relation may be refined. For these structures, there is a basis such that the matrices of the point group belong to the group GL$(3, d, \mathbb{Z})$, the subgroup of the general group GL$(n, \mathbb{Z})$ with matrices of the form

$$\begin{pmatrix}A&v\\0&B\end{pmatrix},$$

where A is a 3×3, v a $d\times 3$ and B a $d\times d$ matrix. Two superspace groups for modulated structures are equivalent if they are conjugate subgroups in the subgroup of the affine group that is the semi-direct product of the translation group and GL(n, d, R).

The superspace groups form a subset of all the nD space groups, but two non-equivalent superspace groups under this equivalence relation may still be isomorphic, and thus equivalent as nD space groups. The (3+1)D superspace groups

Table 10
The space groups for the system $5\bar{3}m(5^2\bar{3}m)$.

Generators	Centring	Symbol
(x, z, u, v, w, y) $(w, x, v, -z, -u, y)$	P_6	$P532(5^232)$
$(x+1/5, z, u+1/5, v, w, y-1/5)$ $(w, x, v, -z, -u, y)$	P_6	$P5_x32(5^232)$
(x, z, u, v, w, y) $(w, x, v, -z, -u, y)$	I_6	$I532(5^232)$
$(x+1/5, z+1/5, u-1/5, v+2/5, w-1/5, y-1/5)$ $(w, x, v, -z, -u, y)$	I_6	$I5_x32(5^232)$
(x, z, u, v, w, y) $(w, x, v, -z, -u, y)$	F_6	$F532(5^232)$
$(x-3/10, z+1/10, u+1/5, v, w-1/5, y-1/5)$ $(w, x, v, -z, -u, y)$	F_6	$F5_x32(5^232)$
(x, z, u, v, w, y) $(w, x, v, -z, -u, y)$ $(-x, -y, -z, -u, -v, -w)$	P_6	$P5\bar{3}m(5^2\bar{3}m)$
$(x, z+1/2, u+1/2, v+1/2, w+1/2, y)$ $(w, x, v, -z, -u, y)$ $(-x, -y, -z, -u, -v, -w)$	P_6	$P5\bar{3}m_{zu}(5^2\bar{3}m)$
(x, z, u, v, w, y) $(w, x, v, -z, -u, y)$ $(-x, -y, -z, -u, -v, -w)$	I_6	$I5\bar{3}m(5^2\bar{3}m)$
(x, z, u, v, w, y) $(w, x, v, -z, -u, y)$ $(-x, -y, -z, -u, -v, -w)$	F_6	$F5\bar{3}m(5^2\bar{3}m)$
$(x, z+1/4, u, v, w+1/4, y+1/2)$ $(w, x, v, -z, -u, y)$ $(-x, -y, -z, -u, -v, -w)$	F_6	$F5\bar{3}m_{z/2u/2}(5^2\bar{3}m)$

Table 11
Space-group symbols for the superspace groups for modulated crystals in (3+1)D for the symmorphic groups of the Bravais groups.

Superspace symbol	Space-group symbol	Equivalent symbol
$P\bar{1}(\alpha\beta\gamma)$	$P_4\overline{1_4}$	
$P2/m(\alpha\beta0)$	$P_4\bar{1}\perp m$	
$P2/m(\alpha\beta\frac{1}{2})$	$I_{zu}\bar{1}\perp m$	
$B2/m(\alpha\beta0)$	$I_{xz}\bar{1}\perp m$	$I_{zu}\bar{1}\perp m$
$P2/m(00\gamma)$	$P_4 2\perp 2$	
$P2/m(\frac{1}{2}0\gamma)$	$I_{xu}2\perp 2$	
$B2/m(00\gamma)$	$I_{xz}2\perp 2$	$I_{xu}2\perp 2$
$B2/m(0\frac{1}{2}\gamma)$	$I_{xz,yu}2\perp 2$	
$Pmmm(00\gamma)$	$P_4 mm\perp 2$	
$Pmmm(0\frac{1}{2}\gamma)$	$I_{yu}mm\perp 2$	$I_{yz}mm\perp 2$
$Pmmm(\frac{1}{2}\frac{1}{2}\gamma)$	$F_{xyu}mm\perp 2$	$F_{xyz}mm\perp 2$
$Immm(00\gamma)$	$I_{xyz}mm\perp 2$	
$Cmmm(00\gamma)$	$I_{xy}mm\perp 2$	
$Cmmm(10\gamma)$	$I_{xyu}mm\perp 2$	$I_{xyz}mm\perp 2$
$Ammm(00\gamma)$	$I_{yz}mm\perp 2$	
$Ammm(\frac{1}{2}0\gamma)$	$I_{yz,xu}mm\perp 2$	
$Fmmm(00\gamma)$	$F_{xyz}mm\perp 2$	
$Fmmm(10\gamma)$	$I_{yz,xyu}mm\perp 2$	$I_{yz,xu}mm\perp 2$
$P4/mmm(00\gamma)$	$P_4 4mm\perp 2$	
$P4/mmm(\frac{1}{2}\frac{1}{2}\gamma)$	$I_{xyu}4mm\perp 2$	$I_{xyz}4mm\perp 2$
$I4/mmm(00\gamma)$	$I_{xyz}4mm\perp 2$	
$R\bar{3}m(00\gamma)$	$R_{xyz}\bar{3}m(m1)$	
$P\bar{3}1m(\frac{1}{3}\frac{1}{3}\gamma)$	$I_{xyu}4mm\perp 2$	$I_{xyz}4mm\perp 2$
$P6/mmm(00\gamma)$	$P_4 6mm\perp m$	

for modulated crystals are given in Janssen, Janner *et al.* (1999). In Table 11, the space-group symbols are given for the symmorphic superspace groups corresponding to the Bravais groups of the (3+1)D space. Superspace groups for 3+*d* dimensions ($d = 1, 2, 3$) can be found on the internet at the web site http://quasi.nims.go.jp/yamamoto/index.html. The Bravais classes for modulated structures in 3+*d* dimensions are given in Janner *et al.* (1983).

A brief introduction to the notation for superspace groups follows. The components of point-group elements and translations in physical space form a 3D space group, with symbol S. In reciprocal space, the diffraction spots can be distinguished as main reflections and satellites. A basis set of satellite vectors may be obtained from a subset $\{\mathbf{q}_1, \ldots, \mathbf{q}_s\}$ by the action of the point group. Finally, each point-group element present in the symbol S may have translation components in the internal (or perpendicular) space symbolized by alpha-numerical characters a. The symbol for the superspace group then is $S(\{\mathbf{q}_1, \ldots, \mathbf{q}_s\})a$. For more details, see *IT* Vol. C (Janssen, Janner *et al.*, 1999). An example of such a symbol is $Pcmn(00\gamma)1s1$, the symbol for a (3+1)D superspace group with component $Pcmn$ in physical space and satellites $\gamma\mathbf{c}^*$. The mirror m in $Pcmn$ accompanies an internal translation $1/2\mathbf{d}$ given by the symbol 's'. The glide planes 'c' and 'n' do not have an associated internal translation. This is given by '1'. Generators for this space-group transform (x, y, z, u) into $(-x+\frac{1}{2}, y, z+\frac{1}{2}, u)$, $(x, -y+\frac{1}{2}, z, u+\frac{1}{2})$ and $(x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{1}{2}, -u)$. This group would be denoted in the recommended notation for nD as $m_z m_u\perp 2P$.

For all quasiperiodic crystals, the nD point group is an R-reducible group with an invariant subspace that has the dimension of the physical space. However, the equivalence of superspace groups may depend on the type of quasi-periodic crystal. Conjugation in the semi-direct product of $T(n)$ and $\mathrm{GL}(n, d, R)$ has been adopted as the equivalence relation for displacively modulated crystals. In the case of composites and quasicrystals, the coarser equivalence of the conjugation in $E(n)$ is used conventionally. In each case, it is evident from the notation that the point group is R-reducible. This notation differs sometimes from that recommended in the present Report for nD space groups. A number of examples are given in Table 12 of superspace groups that are non-equivalent as superspace groups but equivalent as space groups, together with the recommended nD notation.

9. Conclusions and recommendations

Symbols and notation for R-irreducible geometric crystal classes, for arithmetic crystal classes, for Bravais classes and for space groups are discussed in §§2–7, the relation between nD space groups and the symmetry groups for aperiodic crystals in §8. The conclusions can be summarized in the following recommendations.

(I) R-irreducible geometric crystal classes receive a symbol that is composed of symbols for generating subgroups.

Table 12
Some examples of non-equivalent superspace groups that are equivalent as nD space groups.

Superspace group	n n-dimensional space group		Superspace group	n n-dimensional space group
$P2_1(\frac{1}{2}0\gamma)$	4 $I_{xu}2_z$	$\sim$	$Bb(00\gamma)$	4 $I_{xz}2_y$
$Pbnn(\frac{1}{2}\frac{1}{2}\gamma)qq0$	4 $F_{xyu}m_{y/2u/2}m_{x/2u/2z}$	$\sim$	$Fddd(00\gamma)s00$	4 $F_{xyz}m_{y/2z/2}m_{x/2z/2u}$
$P4/mmm(\frac{1}{2}\frac{1}{2}\gamma)$	4 $I_{xyu}4m\perp m$	$\sim$	$I4/mmm(00\gamma)$	4 $I_{xyz}4m\perp m$

(*a*) The full point group is the product of the subgroups. A direct product is given by '×', a general product by a dot '.'.

(*b*) The symbols for the subgroups are those of a generator for a cyclic group, the conventional symbols in 2D and 3D, and the symbols given in Report I.

(*c*) When the symbol of a subgroup is identical to that of an orthogonal transformation but the point group is not the corresponding cyclic group, then the symbol is placed in parentheses.

(*d*) By preference, the subgroups are chosen such that the product of their orders is the order of the point group; otherwise, the order is indicated by a subindex between brackets at the end.

(II) Bravais classes are indicated by the symbol of the geometric crystal class of the holohedry followed by a symbol for the centring.

(*a*) Symbols for nD P-, I-, F- and R-centrings are P_n, I_n, F_n and R_n, respectively.

(*b*) I, F and R centrings of sublattices are given by the same letters, but with the axes of the sublattice involved as a subindex.

(*c*) When I, F or R centrings occur in more than one sublattice, the various sublattices are indicated by the corresponding sets of axes, separated by a comma.

(*d*) When the centring can be considered as the centring of a centred lattice, it is given as a series of centring symbols.

(*e*) Symbols for 4D are given in Table 4.

(III) The symbol for an arithmetic class is the symbol for the geometric class followed by the centring symbol.

(*a*) When the orientation of the point group with respect to the centred basis is relevant, the orientation of the centring is explicitly given.

(*b*) Different orientations of the point group with respect to the lattice are given by indicating the invariant spaces for those group operators for which the orientation matters as a superscript for the corresponding symbol.

(*c*) Mirror operations in an invariant space are given by $\dot{m}$ when the inversion operation is along the projection of a lattice basis vector, by $\ddot{m}$ when it is perpendicular; for 3D components, $N\dot{m}$ is conventionally denoted as $Nm1$ and $N\ddot{m}$ by $N1m$.

(IV) A space group (type) is given by a centring symbol, the symbol for the arithmetic crystal class (but with the centring symbol removed) and by an indication for the intrinsic part of the translation parts of the generators corresponding to the components of the symbol.

(*a*) The intrinsic translation is given as a subindex at the corresponding symbol for the point-group generator.

(*b*) The translation is given with respect to a conventional basis.

(*c*) When N is the order of the orthogonal part, the translations are given as sums of $1/N$ of the basis vectors; the latter are indicated by $x, y, z, u, v, w, \ldots$.

(*d*) To the symbol for the geometrical crystal class are added symbols for new generators if the intrinsic parts associated with the original generators are zero or do not give enough information about the space-group type; for these additional generators, elements are chosen with non-zero intrinsic translation.

(*e*) If necessary, to avoid ambiguity the translation parts of the generators are chosen in such a way that the intrinsic parts are non-zero; this may be done by adding lattice translations of the centring type.

(V) Superspace-group symbols [*IT* Vol. C (Janssen, Janner *et al.*, 1999)] may be used for the symmetry description of incommensurate modulated structures. The full n-dimensional symbol is recommended for incommensurate composites and quasicrystals.

Correction. In Table 3 of I, the symbol $m\bar{4}3m\perp m$ in 19_2 should be $m\bar{3}\perp m$.

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