JOURNAL OF APPLIED CRYSTALLOGRAPHY

ISSN 1600-5767

Received 19 May 2018
Accepted 7 September 2018

Edited by G. J. McIntyre, Australian Centre for Neutron Scattering, Australia

Keywords: space-group classification; crystal classes; crystal systems; crystal families; Bravais classes; lattice systems.

Crystallographic shelves: space-group hierarchy explained

Massimo Nespolo,[a]* Mois Ilia Aroyo[b] and Bernd Souvignier[c]

[a]Université de Lorraine, CNRS, CRM2, Nancy, France, [b]Física de la Materia Condensada, Facultad de Ciencia y Tecnología, Universidad del País Vasco, Apartado 644, Bilbao 48080, Spain, and [c]Institute for Mathematics, Astrophysics and Particle Physics, Faculty of Science, Mathematics and Computing Science, Radboud University Nijmegen, Postbus 9010, Nijmegen 6500 GL, The Netherlands. *Correspondence e-mail: massimo.nespolo@univ-lorraine.fr

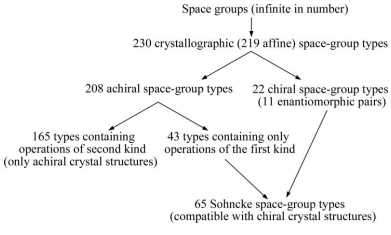
Space groups are classified, according to different criteria, into types, classes, systems and families. Depending on the specific research topic, some of these concepts will be more relevant to the everyday crystallographer than others. Unfortunately, incorrect use of the classification terms often leads to misunderstandings. This article presents the rationale behind the different classification levels.

1. Introduction

A French proverb states that hierarchy is like shelves: the higher they are, the less useful they are. (‘La hiérarchie c’est comme une étagère, plus c’est haut, plus c’est inutile.’) While this may well apply to social sciences, in exact sciences hierarchy is behind fundamental concepts like taxonomy and phylogenetics. Crystallography is no exception: crystal structures and their symmetry groups are arranged in a hierarchical way into classes, systems and families that emphasize common features used as classification criteria. Unfortunately, incorrect definitions and sloppy terminology are not rare in textbooks and scientific manuscripts, and frequently lead to misunderstandings. In this article we present a brief panoramic overview of well known and less well known crystallographic terms in a practical and concrete approach; our aim is also to help the less theoretically inclined crystallographer to understand and apply the concepts expressed by these terms. Our reference is Volume A of *International Tables for Crystallography* (Aroyo, 2016), whose chapters are indicated henceforth as ITA*X* where *X* is the number of the chapter.

For the following discussion we need to remind the reader that, with respect to a coordinate system, a symmetry operation is represented by a matrix–column pair (**W**, **w**), where the (3 × 3) matrix **W** is called the linear or matrix part and the (3× 1) column **w** is the translation or column part. A translation is represented as (**I**, **w**), where **I** is the identity matrix. A rotation, reflection or rotoinversion about the origin is represented by (**W**, **0**), where **0** is the zero column. The column **w** can be decomposed into two components: an **intrinsic** part, which represents the screw or glide component of the operation (screw rotation or glide reflection), and a **location** part, which is non-zero when the rotation axis or reflection plane does not pass through the origin. For example, the matrix–column pair

$$\left(\begin{array}{ccc|c} \overline{1} & 0 & 0 & \frac{1}{2} \\ 0 & 1 & 0 & \frac{1}{2} \\ 0 & 0 & \overline{1} & \frac{1}{2} \end{array}\right)$$



represents an operation mapping a point with coordinates x, y, z to a point with coordinates $\overline{x}+\frac{1}{2}, y+\frac{1}{2}, \overline{z}+\frac{1}{2}$. This is found to be a 180° screw rotation about a line $\frac{1}{4}, y, \frac{1}{4}$, parallel to the b axis but passing through $x=\frac{1}{4}$, $z=\frac{1}{4}$, with an intrinsic (screw) component $\frac{1}{2}$ parallel to b. Depending on whether their intrinsic part is zero or not, symmetry operations are of finite or infinite order. In the former case, the operation is a rotation, reflection or rotoinversion and has at least one fixed point, while in the latter case it is a screw rotation or glide reflection and does not leave any point fixed.

A **symmetry operation** of an object is an isometry (congruence) which maps the object onto itself. Except for the identity and for translations, a **geometric element** is attached to each symmetry operation, which is closely related to the set of fixed points of the operation. Thus, for (glide) reflections and (screw) rotations the geometric elements are planes and lines, respectively. For a rotoinversion, the geometric element is the line of the corresponding rotation axis together with the unique inversion point on the axis fixed by the rotoinversion. Finally, in the case of an inversion, the inversion centre serves as geometric element. A **symmetry element** is defined as the combination of a *geometric element* with the set of symmetry operations having this geometric element in common (the so-called **element set**) (de Wolff *et al.*, 1989, 1992; Flack *et al.*, 2000). Among the symmetry operations sharing the same geometric element, the simplest one [more precisely, the one with the smallest positive (possibly zero) intrinsic translation part] is called the **defining operation** of the symmetry element. It specifies the name (mirror plane, glide plane, rotation axis, screw axis) and the symbol (alphanumeric and graphic) of the symmetry element. For example, consider the geometric element x, y, 0 (a plane) with an element set composed of an infinite number of glide reflections g with glide vectors $(p+\frac{1}{2}, q, 0)$, where p and q are integers. The defining operation corresponds to $p=q=0$ and the symbol g $(\frac{1}{2}, 0, 0)$ x,y,0 is replaced by the special symbol a x,y,0.

The translational symmetry is captured by the *conventional cell*. This is a unit cell that satisfies the three conditions below (ITA1.3.2):

(i) Its basis vectors **a**, **b**, **c** define a right-handed axial setting.

(ii) Its edges are along symmetry directions of the lattice.

(iii) It is the smallest cell compatible with the above conditions.

The metric properties of the conventional cell, and thus also of the translational subgroup, are determined by the cell parameters a, b, c, α, β, γ and are reflected by the **metric tensor**, a square symmetric matrix **G** whose elements are the scalar products of the basis vectors:

$$\mathbf{G}=\begin{pmatrix}\mathbf{a}\cdot\mathbf{a} & \mathbf{a}\cdot\mathbf{b} & \mathbf{a}\cdot\mathbf{c}\\ \mathbf{b}\cdot\mathbf{a} & \mathbf{b}\cdot\mathbf{b} & \mathbf{b}\cdot\mathbf{c}\\ \mathbf{c}\cdot\mathbf{a} & \mathbf{c}\cdot\mathbf{b} & \mathbf{c}\cdot\mathbf{c}\end{pmatrix}=\begin{pmatrix}a^2 & ab\cos\gamma & ac\cos\beta\\ ab\cos\gamma & b^2 & bc\cos\alpha\\ ac\cos\beta & bc\cos\alpha & c^2\end{pmatrix}. \quad (1)$$

2. Group *versus* group type

The first and probably most common confusion that occurs in the literature is the use of the term 'group' for a type of group. A symmetry group is a group (in the algebraic sense) formed by the set of symmetry operations of a given object. In crystallography, the objects are typically atoms, molecules and crystal structures.

A crystal structure is usually described as an idealized periodic pattern of atoms in three-dimensional space using the corresponding coordinates with respect to the chosen coordinate system. Conventionally, these coordinate systems are adapted to the symmetry properties of the crystal structure. For example, the basis vectors are oriented along symmetry directions and display the periodicity of the structure.

The symmetry of two objects is described by *the same group* if the symmetry operations of the first object are also symmetry operations of the second and *vice versa*. However, for different crystal structures this is almost never the case, since a translation bringing one of these structures to overlap with itself will not be a symmetry operation of the other, due to their different cell parameters. On the other hand, after choosing suitable coordinate systems for both structures, the symmetry operations may well be represented by the same matrix–column pairs when expressed in the respective coordinate system. In this case, the space groups of the two crystal structures are said to belong to *the same type*. The difference between space groups and space-group types becomes clear when comparing the symmetry groups of different structures which belong to the same space-group type. For example, jadeite, $NaAlSi_2O_6$, and thoreaulite, $SnTa_2O_7$, are two monoclinic minerals differing in their chemistry, structure, properties and formation environment. To specify the symmetry groups, we also need the cell parameters of the conventional cell, which determine the coordinate system. These are a = 9.418, b = 8.562, c = 5.219 Å and β = 107.58° for jadeite (Prewitt & Burnham, 1966), and a = 17.140, b = 4.865, c = 5.548 Å and β = 91.0° (Mumme, 1970) for thoreaulite. Clearly, applying the translations of one mineral to the other mineral would not bring the structure to coincide with itself and they would thus not be symmetry operations of the second mineral, showing that these two minerals have different space groups. However, when the space groups are expressed with respect to the conventional coordinate systems with basis vectors along the a, b and c axes and with lengths given by the cell parameters, the matrix–column pairs of the symmetry operations become the same and the space groups therefore belong to the same type: $C2/c$ (No. 15). The Hermann–Mauguin symbol [see a recent discussion by Nespolo & Aroyo (2016)] identifies the type of space group, not the space group itself. In everyday laboratory jargon, the word 'type' is often dropped and this does not normally impede the transmission of information. In other cases, like the classifications we are going to discuss below, or in the context of group–subgroup relations, the difference is of paramount importance. For example, a single space group may have various different subgroups of the same type which can correspond to different phase transitions, or to different domain states arising in a phase transition. In any

Table 1
Metric tensors of the 14 types of Bravais lattices with respect to the conventional bases.

Being symmetric with respect to the main diagonal, the metric tensor is shown as an upper-triangular matrix. The non-zero elements of the metric tensor correspond to the free parameters of the respective Bravais lattice types. See also Table 3.1.2.2 in ITA.

Cell parameters of the conventional cell	Metric tensor of the conventional cell	Bravais type of lattice	Symmetry of the lattice (holohedry)
$a, b, c, \alpha, \beta, \gamma$	$\begin{matrix} g_{11} & g_{12} & g_{13} \\ & g_{22} & g_{23} \\ & & g_{33} \end{matrix}$	aP	$\bar{1}$
a, b, c, β; $\alpha = \gamma = 90^\circ$	$\begin{matrix} g_{11} & 0 & g_{13} \\ & g_{22} & 0 \\ & & g_{33} \end{matrix}$	mP, mS (b unique)	$2/m$
a, b, c, $\alpha = \beta = \gamma = 90^\circ$	$\begin{matrix} g_{11} & 0 & 0 \\ & g_{22} & 0 \\ & & g_{33} \end{matrix}$	oP, oS, oI, oF	mmm
$a = b$; c, $\alpha = \beta = \gamma = 90^\circ$	$\begin{matrix} g_{11} & 0 & 0 \\ & g_{11} & 0 \\ & & g_{33} \end{matrix}$	tP, tI	$4/mmm$
$a = b$; c, $\alpha = \beta = 90^\circ$; $\gamma = 120^\circ$	$\begin{matrix} g_{11} & -g_{11}/2 & 0 \\ & g_{11} & 0 \\ & & g_{33} \end{matrix}$	hR	$\bar{3}m$
$a = b$; c, $\alpha = \beta = 90^\circ$; $\gamma = 120^\circ$	$\begin{matrix} g_{11} & -g_{11}/2 & 0 \\ & g_{11} & 0 \\ & & g_{33} \end{matrix}$	hP	$6/mmm$
$a = b = c$, $\alpha = \beta = \gamma = 90^\circ$	$\begin{matrix} g_{11} & 0 & 0 \\ & g_{1} & 0 \\ & & g_{11} \end{matrix}$	cP, cI, cF	$m\bar{3}m$

case, one should bear in mind that the number of space-group types is finite, whereas that of space groups is infinite, due to the infinitely many possible values for the cell parameters and for the orientation and location in space of the geometric elements.

The type of a lattice is characterized by a number of free parameters, which correspond to the symmetry-unrestricted cell parameters and are represented by the independent non-zero elements of the metric tensor (Table 1). It is often overlooked that, while the presence of certain symmetry operations of the crystal structure can restrict the possible ratios of cell lengths or angular values, their absence cannot impose any restriction. Although this should be self-evident, textbooks often define a type of Bravais lattice by imposing that some cell parameters are *not* identical to each other or to a certain value. For example, a tetragonal lattice is often defined as having $a \neq c$, while a and c, being symmetry *un*restricted, can take *any* value, including the special case $a = c$. This equality is realized within the standard uncertainty of the experiment and holds within a certain interval of temperature and pressure [see a detailed discussion by Nespolo (2015*b*)]. In that case, one speaks of **metric specialization** (or **specialized metric**), a phenomenon more frequent than is commonly thought (Janner, 2004*a*,*b*) that may severely hinder the structure solution and refinement strategy and which increases the frequency of occurrence of twinning (Nespolo & Ferraris, 2000). Metric specialization prevents the direct classification of space groups based merely on the cell parameters. In fact, two space groups of the same type, one with and the other without metric specialization, have lattices of different symmetry (cubic and tetragonal in the example above). It would, however, be unreasonable to assign these two space groups to different categories (classes, systems, families), because the metric specialization is often an 'accident', not a feature of the structure crystallizing in that group. The higher symmetry of the translation subgroup (and thus of the unit cell) is broken by the contents of the unit cell which allows only a symmetry group of the lower type. Thus, to apply a consistent classification scheme, we have to abstract from any metric specialization. For this reason, the classification scheme is applied to space-group types, not to space groups (ITA1.3.4). We further discuss the consequences of metric specialization in §§5 and 7.

The same distinction between groups and types of groups must also be made for point groups. The common statement that there are 32 crystallographic point groups (in three-dimensional space) is again, strictly speaking, incorrect because it actually applies to point-group types. As already seen in the case of space groups, point groups too are infinite in number, because of the infinitely many possible orientations in space of the geometric elements. Point groups are represented by matrices with respect to a chosen basis of the underlying vector space and, similar to space groups, two point groups belong to the same type if their matrices can be made to coincide by choosing suitable bases. Again, the bases are usually chosen in a symmetry-adapted way and the transformation between two bases captures the relative orientation of the two point groups. The relative orientation of point groups is crucial to the analysis of general domain structures, in particular for growth twins (Nespolo, 2015*a*). A finer classification into 136 classes of *oriented* point groups takes into account the orientation of the symmetry elements with respect to a reference coordinate system and is obtained by considering the subgroups of the cubic and hexagonal holohedries (Nespolo & Souvignier, 2009; holohedry indicates the full symmetry of a lattice: see §6 for a precise definition): these classes are of particular importance in the study of domain structures obtained following a phase transition. For example, a cubic crystal with point group of type $4/m\bar{3}2/m$ ($m\bar{3}m$) that undergoes a phase transition to $4/m2/m2/m$ ($4/mmm$) retains one of the three fourfold axes of the cubic parent phase. It can be oriented along the cubic a, b or c axes, leading to three differently oriented but isomorphic groups of type $4/mmm$.

The difference between point groups and point-group types is the key to the classification of space groups into geometric crystal classes. The term 'space group' (not hyphenated) should be used with reference to a given crystal structure, while the term 'space-group type' (hyphenated) should instead be used when speaking in general of the type of

symmetry common to all crystal structures whose space groups only differ in the values of their cell parameters.

3. Chirality and handedness. Sohncke, affine and crystallographic space-group types

The symmetry group of a crystal structure (*i.e.* its space group) can be regarded as an object: if we look at a space-group diagram as a geometric figure, we can observe how its symmetry elements are distributed in space and find isometries that map those symmetry elements onto each other. In other words, we can find the symmetry group of that drawing. The symmetry operations of an object are isometries (Euclidean mappings), *i.e.* transformations that do not deform the object and form a group: the symmetry group of that object. The symmetry group depends on the type of object under consideration: for molecules, it is a point group, and for crystal structures, it is a space group. For a space-group symmetry-element diagram regarded as a geometric figure, the symmetry is described by the Euclidean normalizer (or Cheshire group); it is also termed the 'symmetry of the symmetry' because it maps the symmetry elements of the space group onto themselves (possibly permuting them) (Koch & Fischer, 2006).

When considering symmetry operations, one distinguishes whether an operation maps a right-handed coordinate system to a right-handed one or a left-handed one. The former, rotations, screw rotations and translations, are called orientation-preserving, or operations of the first kind: they are characterized by the fact that their linear part has determinant +1. In contrast, reflections, glide reflections, rotoinversions and inversions are called orientation-reversing or operations of the second kind: their linear parts have determinant −1. Only operations of the first kind can be applied to real objects in physical space. Every operation of the second kind can be obtained as an operation of the first kind followed by an inversion.

An object is said to be **chiral** if it cannot be superimposed on its mirror image by an operation of the first kind; the two non-superimposable mirror images of a chiral object are said to possess opposite **handedness** (left or right). The symmetry group of a chiral object contains only operations of the first kind; if it contained any operation of the second kind, the composition of this operation with a reflection mapping the object to its mirror image would result in an operation of the first kind mapping it to its mirror image, thus making the object achiral. If the chiral object under consideration is a crystal structure, the two variants with opposite handedness are called **enantiomorphs** and their space groups belong to one of the 65 types containing only operations of the first kind, called **Sohncke space-group types** [after the German mathematician Leonhard Sohncke (1842–1897)].

Sohncke groups are often *incorrectly* called 'chiral groups', so the difference between these two concepts needs to be clarified. Sohncke groups are groups representing the possible symmetry of chiral *objects*, but the groups themselves are not necessarily chiral. The difference between the chirality of an object and the chirality of a symmetry group is, unfortunately, sometimes overlooked (Flack, 2003). There is, indeed, a certain similarity between the two concepts. As we have seen, for a chiral object the symmetry group of the object as a whole is required to consist only of symmetry operations of the first kind. Similarly, a group is called chiral if its Euclidean normalizer contains only operations of the first kind. In this case it has a counterpart of opposite handedness which belongs to a different space-group type; the two groups then form an enantiomorphic pair and differ by the presence of screw rotations of the same type but turning in opposite directions, like $P3_1$ and $P3_2$. Twenty-two types of space groups are chiral and form 11 pairs of enantiomorphic space-group types; the other 208 types are achiral. Chiral space-group types are Sohncke types because a space group is contained in its Euclidean normalizer, but the opposite is not true: 43 of the 65 Sohncke types are not chiral. For example, space-group types $P4_1$ (No. 76) and $P4_3$ (No. 78) are chiral and form an enantiomophic pair; they obviously belong to the Sohncke type of groups. On the other hand, the Sohncke type $P4_2$ (No. 77) is *not* chiral: it does not have an enantiomorphic counterpart because its Euclidean normalizer also contains operations of the second kind (*e.g.* the inversion at the origin).

Summarizing, to distinguish between achiral and chiral types of space groups it is sufficient to check whether their Euclidean normalizers do or do not contain operations of the second kind, in exactly the same way as we distinguish between achiral and chiral crystal structures by checking whether their space groups do or do not contain operations of the second kind.

When considered from a more abstract algebraic viewpoint, space-group types belonging to an enantiomorphic pair are not distinguished: they have the same group structure and the symmetry operations in these groups are either identical or differ only for the direction of a screw rotation, like in the case of 3_1 and 3_2. Depending on whether enantiomorphic space-group types are considered as different (as crystallographers usually do) or not (as mathematicians usually do), we obtain 230 *crystallographic* or 219 *affine* types of space groups. Fig. 1 summarizes the classification of space-group types in terms of

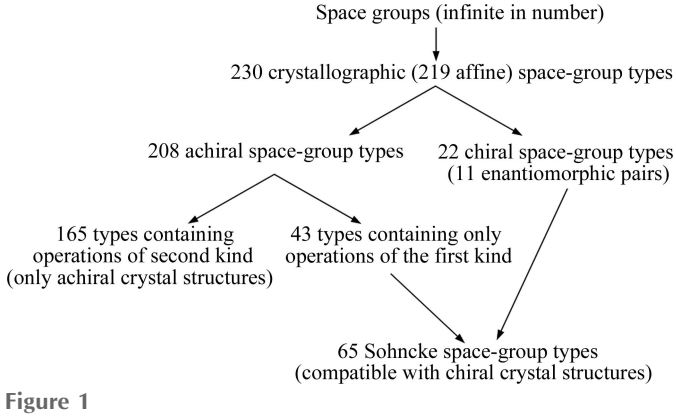


Figure 1
Classification of space groups into chiral and achiral types, and into Sohncke types and space-group types containing operations of the second kind.

the chirality of the groups and of the structures crystallizing in them.

4. Symmorphic types of space groups and arithmetic crystal classes

A space group is characterized by its group of linear parts, *i.e.* its point group, its translation lattice, represented by the unit cell, and the translational parts of its generators, which reflect the interplay between the point group and the translation lattice. In order to proceed to the higher shelves in the classification hierarchy of space groups, part of the information on point groups, translation lattices and their interplay is ignored and groups are collected together when they coincide only on a part of these aspects. Keeping the information on the point group and translation lattice, but neglecting their interplay, leads to the concept of symmorphism [see a recent analysis by Nespolo (2017)] and to the classification into arithmetic crystal classes. Before proceeding, we need to recall the concept of a **site-symmetry group**, which is a subgroup of the space group G containing all the symmetry operations in G that leave a point (the 'site') fixed.

A space group is said to be symmorphic if a coordinate system can be chosen such that all the non-translation generators have zero translational part. As a consequence, the site-symmetry group of the origin of this coordinate system is isomorphic to the point group, *i.e.* the group of linear parts occurring in the space group. For a non-symmorphic space group, the order of the site-symmetry group of each point (or the corresponding Wyckoff position) is a proper divisor of the order of the point group.

A symmorphic space-group type is easily recognized from its Hermann–Mauguin symbol by the fact that, apart from the letter indicating the centring mode, it coincides with a point-group symbol. In particular, it only contains the symbols 1, 2, 3, 4, 6 for rotations, $\overline{1}$, $\overline{3}$, $\overline{4}$, $\overline{6}$ for rotoinversions, and m for reflections. This does *not* necessarily mean that a symmorphic group does not include glide planes or screw axes, as is sometimes incorrectly stated in the literature. For example, a symmorphic space group of type $C222$ (No. 21) contains screw axes parallel to the a and b axes, which are obtained by composing rotations along the a and b axes with the centring translation.

The role of symmorphic space groups in the description of the symmetry of reciprocal space is well established (Wintgen, 1941; Aroyo & Wondratschek, 1995), but for our purposes the symmorphic types of space groups form the basis for further classification of space groups.

Each space-group type is associated with a unique symmorphic type. Starting with non-translation generators of the space group, one simply changes their translational parts to zero, and the space group generated by these modified generators (and the translations of the original group) is then symmorphic by definition. Moreover, the Hermann–Mauguin symbol of the associated symmorphic type can immediately be read off from that of the given space-group type: replace every screw-axis symbol by the corresponding rotation-axis symbol (*e.g.* 3_1 by 3) and every glide-plane symbol a, b, c, d, e, n by the mirror-plane symbol m. All space-group types corresponding to the same symmorphic type are gathered into the same **arithmetic crystal class**, which is identified by the symbol of the corresponding symmorphic type. To avoid any possible confusion, the symbol for the arithmetic crystal class is a modified version of that for the symmorphic space-group type, with the letter indicating the centring type moved from the first position to the last. For example, the arithmetic crystal class corresponding to the space group of type $C222$ is denoted by $222C$. Because there are 73 symmorphic types of space groups, there are also 73 arithmetic crystal classes.

Here the conceptual difference between a group and a class has to be emphasized. A symmetry group is a set of isometries that expresses the symmetry of an object. A class is a set of objects having a common feature with respect to a classification criterion. In the case of arithmetic crystal classes, we gather into the same class those objects (space groups, space-group types, crystal structures) which correspond to the same type of symmorphic space group. A class can be imagined as a shelf where objects (groups, crystal structures, molecules) sharing a common feature are stored. The same conceptual difference occurs again between geometric crystal classes and types of point groups (see §6).

Characterizing symmorphic space groups by the property that they contain site-symmetry groups which are isomorphic to their point groups, one can look at the other extreme, namely space groups in which all site-symmetry groups are trivial, *i.e.* space groups with no special Wyckoff positions. These groups are called **Bieberbach groups** [after the German mathematician Ludwig Georg Elias Moses Bieberbach (1886–1982)] (or **fixed-point-free space groups** or **torsion-free space groups**) and they contain (except for the identity) only operations of infinite order: screw rotations, glide reflections and translations. Of the 230 crystallographic space-group types, 13 are Bieberbach types of groups.

5. Bravais types of lattices, Bravais arithmetic classes and Bravais classes

The symmetry of a structure built by atoms occupying the nodes of a lattice is an example of a symmorphic space-group symmetry: the space group has not only the given lattice as its translation subgroup, as usual, but also the full symmetry group of the lattice as its point group. The arithmetic crystal class containing such a symmorphic group is called a **Bravais arithmetic crystal class** and, by construction, these classes are in one-to-one correspondence with the 14 Bravais types of lattices. If a symmorphic space group does not belong to a Bravais arithmetic crystal class, its point group is not the full symmetry group of a lattice. In that case, the point group can be extended to a unique supergroup of minimal index expressing the full symmetry of the lattice (holohedral supergroup) by adding missing lattice symmetries such that the enlarged symmorphic group belongs to a Bravais arithmetic crystal class. For example, a symmorphic space group of type $P\overline{4}m2$ (No. 115) has a point group of type $\overline{4}m2$ which is

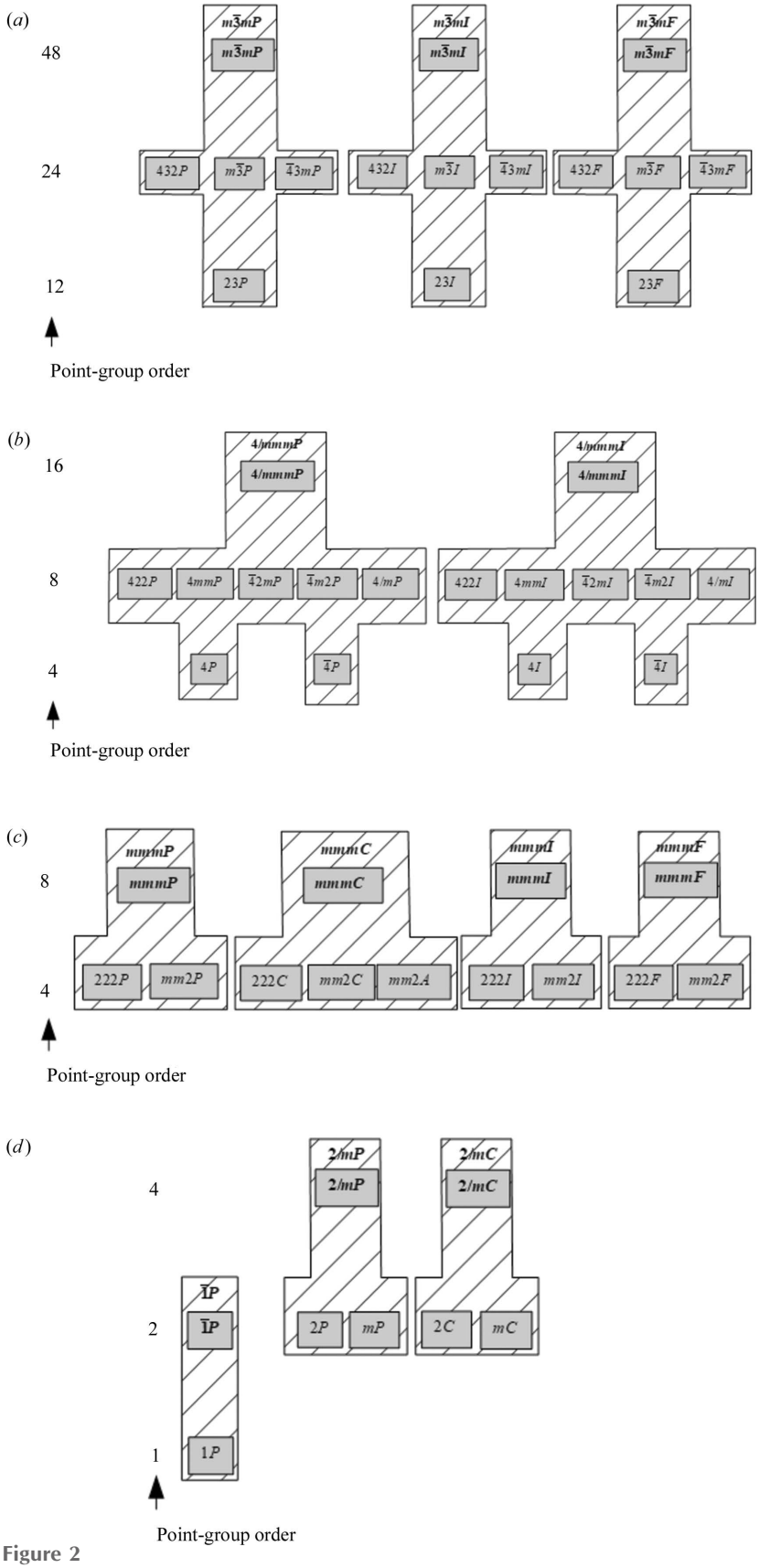


Figure 2
The Bravais classes (striped boxes) obtained from the (*a*) cubic, (*b*) tetragonal, (*c*) orthorhombic, and (*d*) monoclinic and triclinic holohedries. Grey boxes are arithmetic crystal classes. Bold font indicates the symbols of Bravais arithmetic crystal classes; the same symbols are used to specify the Bravais classes.

not the full symmetry group of a lattice, but which is contained (as a subgroup of index 2) in a point group of type 4/*mmm*, the full symmetry group of a tetragonal lattice. Extending the point group to 4/*mmm* gives rise to the symmorphic space group of type *P*4/*mmm* (No. 123) that does belong to the Bravais arithmetic crystal class with symbol 4/*mmmP*. Note that by choosing a minimal holohedral supergroup of the point group, the problem of metric specialization is circumvented. It does not matter whether the translation lattice of the symmorphic group of type $P\bar{4}m2$ is tetragonal or, accidentally, cubic; since the point-group type 4/*mmm* is already a full symmetry group of a lattice one does not consider possible higher symmetries of a cubic lattice. In the way just described, every symmorphic space-group type, and thus also every arithmetic crystal class, is assigned to a Bravais arithmetic crystal class and thus at the same time to a Bravais type of lattice.

Recalling how we collected space-group types into arithmetic crystal classes in the previous section, and combining this with the assignment of an arithmetic crystal class to a Bravais arithmetic crystal class described above, we arrive at an assignment of space-group types to a unique Bravais arithmetic crystal class and thus also to a unique Bravais type of lattice. Two space-group types corresponding to the same Bravais type of lattice are also said to belong to the same **Bravais class**, and one uses the same names and symbols for the Bravais classes as for the Bravais types of lattices. For example, the space-group types $P\bar{4}m2$, $P\bar{4}c2$, $P\bar{4}b2$, $P\bar{4}n2$ (Nos. 115–118) all belong to the same arithmetic crystal class $\bar{4}m2P$ and are, as explained above, assigned to the Bravais arithmetic crystal class 4/*mmmP* and thus belong to the Bravais class of primitive tetragonal type. The other arithmetic crystal classes belonging to this Bravais class are 4*P*, $\bar{4}P$, 4/*mP*, 422P, 4*mmP*, $\bar{4}2mP$ and 4/*mmmP*, and thus all space-group types belonging to any of these arithmetic crystal classes are associated with the primitive tetragonal lattice type. As a synonym for Bravais classes, the term *Bravais flocks* is occasionally used (for example, ch. 8.2 of the 5th edition of *International Tables of Crystallography*, Vol. A. Usually, it is applied to the matrix groups representing the point groups rather than to the space groups.

Figs. 2–4 present a detailed classification of arithmetic crystal classes in Bravais arithmetic crystal classes and Bravais classes.

6. Geometric crystal classes, holohedries and Laue classes

We have seen that by grouping together all the space-group types that correspond to the same symmorphic type we get a set of space-group types called an arithmetic crystal class. Going one step further and fully neglecting the information on the translation subgroup by collecting all space-group types for which the point groups are of the same type, we arrive at a **geometric crystal class**. Because there are 32 types of point groups, by gathering space-group types according to their point-group type we obtain 32 geometric crystal classes. These classes are denoted by the same Hermann–Mauguin symbol as the corresponding point-group types, which is sufficient, since the translation subgroup is ignored and thus is not required to be represented by a symbol as is the case for arithmetic crystal classes. In particular, space-group types differing only by the centring mode of their conventional cell belong to the same geometric crystal class. The double use of the Hermann–Mauguin symbol for point-group types and geometric crystal classes does not give rise to misunderstandings, because from the context it will always be clear which of the two is meant.

The 11 geometric crystal classes corresponding to point-group types that contain only operations of the first kind (1, 2, 3, 4, 6, 222, 422, 32, 622, 23, 432) have been called 'enantiomorphous classes' (Shuvalov, 1988) because they are compatible with chiral crystal structures, which can occur in two enantiomorphous modifications. As we have seen in §3, space groups that belong to these classes are known as Sohncke groups; it would be a logical extension to use the terms *Sohncke crystal classes* and *Sohncke types of point groups*, but to the best of our knowledge the name *Sohncke* has so far only been used for space groups.

Those geometric crystal classes whose members (*i.e.* space-group types) show the full symmetry of a lattice are called **holohedries**. A holohedry is therefore not a group, but a class. A *holohedral* group is a (point or space) group which belongs to a holohedral class; the others are called **merohedral**. Those geometric crystal classes whose members (groups) are centrosymmetric are called *Laue classes*. A Laue class contains all the centrosymmetric space-group types that correspond to the same point-group type. For example, the Laue class 2/*m* contains six space-group types: *P*2/*m*, *P*2$_1$/*m*, *P*2/*c*, *P*2$_1$/*c*, *C*2/*m* and *C*2/*c*.

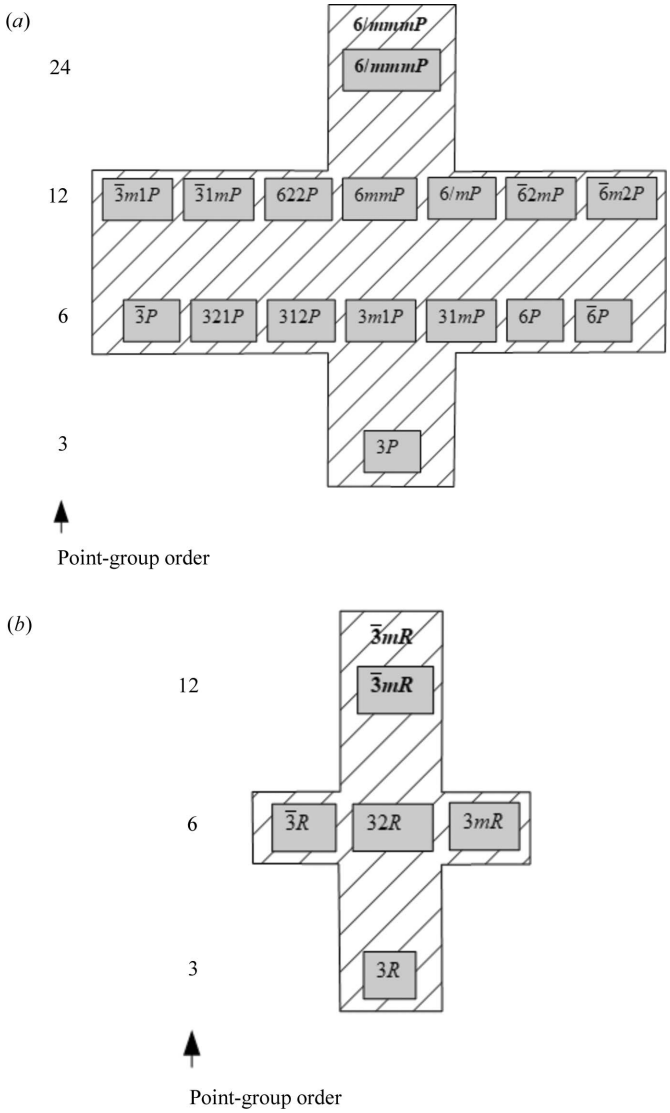


Figure 3
Bravais classes obtained from the (*a*) hexagonal and (*b*) rhombohedral holohedries. The figure uses the same conventions as in Fig. 2.

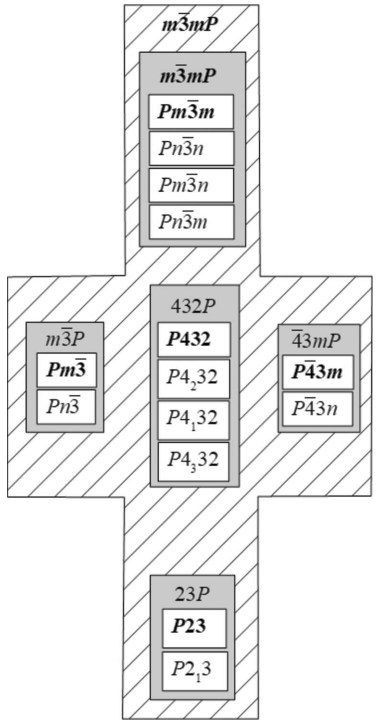


Figure 4
Detailed content of the primitive cubic Bravais class in terms of arithmetic crystal classes (grey) and space-group types (white). The Hermann–Mauguin symbol of the symmorphic groups specifying the arithmetic classes and the symbols of the Bravais arithmetic crystal classes are given in bold.

Table 2
The 32 crystallographic types of point groups and their action on the 14 types of Bravais lattices in three-dimensional space.

Holohedral point-group types are shown in bold font. When a type of point group acts on a type of lattice the corresponding intersection is marked by a tick symbol (√). Point-group types with the same entries are gathered into the same crystal system. Note that the action on lattice types of minimal symmetry, *i.e.* with a maximal number of free parameters, is already sufficient to determine the crystal system.

Point-group types	*aP*	*mP*	*mS*	*oP*	*oS*	*oI*	*oF*	*tP*	*tI*	*hR*	*hP*	*cP*	*cI*	*cF*	Crystal system
1, $\bar{1}$	√	√	√	√	√	√	√	√	√	√	√	√	√	√	Triclinic
2, *m*, **2/*m***		√	√	√	√	√	√	√	√	√	√	√	√	√	Monoclinic
222, *mm*2, ***mmm***				√	√	√	√	√	√		√	√	√	√	Orthorhombic
4, $\bar{4}$, 422, $\bar{4}2m$, 4/*m*, 4*mm*, **4/*mmm***								√	√			√	√	√	Tetragonal
3, $\bar{3}$, 3*m*, 32, $\bar{3}$***m***										√	√	√	√	√	Trigonal
6, $\bar{6}$, 622, $\bar{6}2m$, 6/*m*, 6*mm*, **6/*mmm***											√				Hexagonal
23, $m\bar{3}$, 432, $\bar{4}3m$, $\boldsymbol{m\bar{3}m}$												√	√	√	Cubic
No. of free parameters	6	4	4	3	3	3	3	2	2	2	2	1	1	1	

Point-group types that are compatible with the existence of polar or axial vectors are of particular importance for the study of the physical properties of crystals. A vector is characterized by its magnitude and its direction, and the direction is in turn characterized by an orientation and a sense. The orientation is specified by the relationship between the vector and the reference. The sense is specified by the order of two points either on a line parallel to the vector (polar vector or true vector) or on a loop perpendicular to the vector (axial vector or pseudovector). A polar vector has symmetry ∞m and can be represented by a stationary cone or arrow, whereas an axial vector has symmetry ∞/m and can be represented by a cylinder rotating about its axis.

Point groups compatible with the existence of one polar vector belong to ten *pyroelectric* (or polar) geometric crystal classes, because crystals in these classes can show pyroelectricity. The ten pyroelectric geometric crystal classes are 1, 2, 3, 4, 6, *m*, *mm*2, 3*m*, 4*mm* and 6*mm*. These correspond to the ten point-group types (because of the 1:1 correspondence between point-group types and geometric crystal classes) which are subgroups of the group ∞m. The number of crystallographic space-group types that belong to these pyroelectric geometric crystal classes is 68, which includes four pairs of enantiomorphic space-group types. The presence of a polar vector along a fixed direction, or parallel to a plane (point group of type *m*) or arbitrarily oriented (point group 1), implies that the choice of the origin is not fixed by symmetry but can be taken anywhere along the polar direction. When performing the refinement of a structure crystallizing in a pyroelectric space group, the origin should be fixed by the user [by restraining a centre of mass or fixing the coordinate(s) of one atom along the polar direction], otherwise a large number of correlations result, precisely because of the infinitely many possible choices for the origin.

In an analogous way, ferromagnetic materials can crystallize in point-group types and space-group types that are compatible with the existence of one axial vector. These are the crystallographic subgroups of ∞/m, *i.e.* 1, 2, 3, 4, 6, $\bar{1}$, *m*, 2/*m*, $\bar{3}$, $\bar{4}$, 4/*m*, $\bar{6}$ and 6/*m*. The number of crystallographic space-group types that belong to the corresponding 13 geometric crystal classes is 44, which includes four pairs of enantiomorphic space-group types.

7. Crystal systems

Space-group types are gathered into the same crystal system when their point groups act on (*i.e.* leave invariant) the same types of Bravais lattices. If H and G are point groups and H is a subgroup of G, then H acts on the same types of Bravais lattices as G, but possibly also on other lattice types with more free parameters, whereas the opposite is not necessarily true. For example, 4/*mmm* acts on tetragonal and cubic lattices, and *mmm*, which is a subgroup of 4/*mmm*, acts on tetragonal and cubic lattices as well. However, *mmm* also acts on orthorhombic lattices, on which 4/*mmm* does not act. The action on different types of lattices is the criterion to classify point-group types (and therefore also space-group types) into crystal systems.

Table 2 shows the lattices on which the point-group types act. A crystal system is the shelf on which we can gather all the point-group types (and the corresponding space-group types) which act on the same types of lattices, *i.e.* which have an identical intersection of rows and columns in Table 2. This criterion of acting on the same types of lattices classifies space-group types into seven crystal systems: triclinic (or anorthic), monoclinic, orthorhombic, tetragonal, trigonal, hexagonal and cubic.

It is a common misunderstanding to establish a direct relation between the cell parameters of the conventional cell and the crystal system. Although the cell parameters are a useful indicator, this relation works in general only in the opposite direction: symmetry imposes restrictions on the cell parameters, but absence of symmetry does not. For example, in the case of an orthorhombic crystal (*i.e.* a crystal with a space group belonging to the orthorhombic crystal system), three of the six cell parameters vary independently and, in a certain interval of temperature and pressure, they might take values that correspond to a more symmetric lattice, within the standard uncertainty of the experiment; as discussed above, this is a case of metric specialization. Table 2 shows that point-group types 222, *mm*2 and *mmm* act not only on orthorhombic but also on tetragonal, hexagonal and cubic lattices. If one adopts the cell parameters as a criterion to estimate the structural symmetry, in the case of metric specialization one might be tempted to assign the sample to the tetragonal, hexagonal or cubic crystal system, because the *lattice* of that

sample is tetragonal, hexagonal or cubic. However, the point group unambiguously shows that the *structure* is still orthorhombic.

8. Lattice systems

A space group can be assigned to a unique holohedry by looking for the holohedry of minimal order that contains the point group of the space group and contains the full symmetry of the lattice type of the space group. Grouping together all space groups that are associated with the same holohedry in this way gives rise to the classification of space-group types into lattice systems. For example, space groups of types *P*23, *Im*$\bar{3}$ and *F*432 are all assigned to the *m*$\bar{3}$*m* holohedry and belong to the cubic lattice system. Similarly, space groups of types *P*32 and *P*622 correspond to the 6/*mmm* holohedry and belong to the hexagonal lattice system. On the other hand, space groups of types *R*32 and *P*622 correspond to the different holohedries $\bar{3}m$ and 6/*mmm*, respectively; a group of type *R*32 belongs to the rhombohedral lattice system, whereas *P*622 belongs to the hexagonal lattice system.

Using the classification into Bravais classes as an intermediate step, the lattice systems have a fairly simple description: two Bravais classes belong to the same lattice system if the corresponding Bravais arithmetic classes belong to the same holohedry. This criterion classifies space-group types into seven lattice systems (formerly known as Bravais systems): triclinic (or anorthic) (holohedry $\bar{1}$), monoclinic (2/*m*), orthorhombic (*mmm*), tetragonal (4/*mmm*), rhombohedral ($\bar{3}m$), hexagonal (6/*mmm*) and cubic (*m*$\bar{3}$*m*).

As in the case of crystal systems, a metric specialization can affect the lattice of a particular sample but not its lattice system.

9. Crystal families

The highest shelf in our classification is that of crystal families. Space-group types are gathered into the same crystal family when they correspond to holohedries that are in a group–subgroup relation (Fig. 5) and their types of Bravais lattices have the same number of free parameters. For example, space-group types with holohedries 4/*mmm* and 6/*mmm* have lattices with two free parameters (*a* and *c*; see Table 1). However, 4/*mmm* and 6/*mmm* are not in a group–subgroup relation and thus the corresponding space-group types belong to different crystal families (tetragonal and hexagonal, respectively). On the other hand, space-group types with holohedries $\bar{3}m$ and 6/*mmm* have lattices with two free parameters (*a* and *c* in hexagonal axes) and a point group of type 6/*mmm* contains a subgroup of type $\bar{3}m$. Therefore, the two space-group types belong to the same crystal family (hexagonal).

This criterion classifies space-group types into six crystal families, indicated with a lower-case letter as follows: *a* (anorthic = triclinic), *m* (monoclinic), *o* (orthorhombic), *t* (tetragonal), *h* (hexagonal) and *c* (cubic). The Bravais types of lattices are then indicated by the symbol of the crystal family followed by the centring symbol of the conventional cell, in upper case (*aP*, *mP*, *mC*, *oP*, *oC*, *oI*, *oF*, *tP*, *tI*, *hR*, *hP*, *cP*, *cI*, *cF*; *S* for side-face centred is also used to indicate centring of one face, when one abstracts on whether it is *A*, *B* or *C*).

For five of the six crystal families, the crystal family coincides with a lattice system and a crystal system. However, the hexagonal crystal family is subdivided into two lattice systems (rhombohedral and hexagonal) and into two crystal systems (trigonal and hexagonal). The distribution of space-group types in the hexagonal crystal family over crystal systems and lattice systems is shown in Table 3. Space-group types corresponding to the hexagonal crystal system have an *hP* lattice, whereas space-group types corresponding to the trigonal crystal system may have an *hR* or *hP* lattice. The term *trigonal* indicates that the groups belonging to this crystal system act on both *hR* and *hP* lattice types and has no meaning with reference to lattices. Thus, the term 'trigonal lattice', used in various textbooks, is incorrect. Similarly, the term 'rhombohedral' can not be used with reference to crystal systems, since it applies only to a lattice: the term 'rhombohedral crystal

Table 3
Distribution of space-group types in the hexagonal crystal family (see Table 1.3.4.3 in ITA1.3.4).

		Lattice system	
Crystal system	Geometric crystal class	Hexagonal	Rhombohedral
Hexagonal	6	*P*6, *P*6$_1$, *P*6$_2$, *P*6$_3$, *P*6$_4$, *P*6$_5$	
	$\bar{6}$	*P*$\bar{6}$	
	622	*P*622, *P*6$_1$22, *P*6$_2$22, *P*6$_3$22, *P*6$_4$22, *P*6$_5$22	
	$\bar{6}2m$	*P*$\bar{6}2m$, *P*$\bar{6}2c$, *P*$\bar{6}m2$, *P*$\bar{6}c2$	
	6/*m*	*P*6/*m*, *P*6$_3$/*m*	
	6*mm*	*P*6*mm*, *P*6*cc*, *P*6$_3$*mc*, *P*6$_3$*cm*	
	6/*mmm*	*P*6/*mmm*, *P*6/*mcc*, *P*6$_3$/*mcm*, *P*6$_3$/*mmc*	
Trigonal	3	*P*3, *P*3$_1$, *P*3$_2$	*R*3
	$\bar{3}$	*P*$\bar{3}$	*R*$\bar{3}$
	3*m*	*P*3*m*1, *P*3*c*1, *P*31*m*, *P*31*c*	*R*3*m*, *R*3*c*
	32	*P*321, *P*312, *P*3$_1$21, *P*3$_1$12, *P*3$_2$21, *P*3$_2$12	*R*32
	$\bar{3}m$	*P*$\bar{3}$*m*1, *P*$\bar{3}$*c*1, *P*$\bar{3}$1*m*, *P*$\bar{3}$1*c*	*R*$\bar{3}$*m*, *R*$\bar{3}$*c*

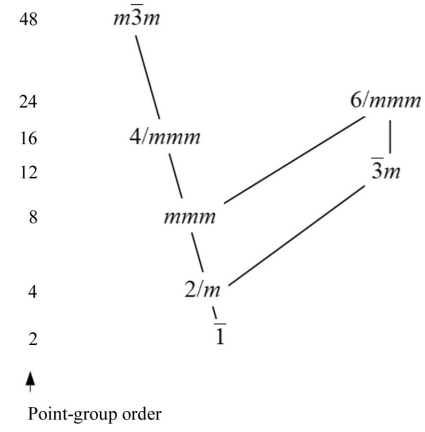


Figure 5
Subgroup tree for the holohedral point-group types.

Table 4
Summary of common errors found in the crystallographic literature and often used in everyday crystallographic jargon.

Incorrect term or expression	Correct use	Remarks
Space group (without reference to a specific crystal structure)	Space-group type	There are infinitely many space groups that belong to the same space-group type. Their common feature is that their symmetry operations can be made to coincide when expressed with respect to a suitable coordinate system. The coordinate systems – and with them the space groups – differ depending on the cell parameters of the specific crystal structures.
Chiral group (when making reference to a chiral crystal structure)	Sohncke group	A chiral crystal structure can occur in any of the 65 Sohncke types of space groups, not only in the 22 chiral types of space groups.
Rhombohedral crystal system	Trigonal crystal system	The term 'rhombohedral' indicates a type of lattice; a crystal with a rhombohedral lattice belongs to the trigonal crystal system.
Trigonal lattice	Rhombohedral lattice	The term 'trigonal' indicates a crystal with a single threefold axis. Its lattice can be either rhombohedral or hexagonal.
Symmetry element (when speaking of the point, line or plane left invariant by a symmetry operation)	Geometric element	A point, line or plane is a geometric element. The combination of a geometric element with the set of all symmetry operations having this element in common is defined as a symmetry element.
A symmorphic space group does not contain screw axes or glide planes	The Hermann–Mauguin symbol of a symmorphic space group does not show the presence of screw axes or glide planes†	The symmetry elements that are shown in the Hermann–Mauguin symbol follow a priority rule, which for symmetry planes is $m > e > a, b, c > n$ and for symmetry axes with the same rotational component prefers rotation axes to screw axes. Accordingly, the symbol of space-group type No. 65 is *Cmmm* (short symbol) or *C*2/*m*2/*m*2/*m* (full symbol), yet twofold screw axes do exist along the [100] and [010] directions, *b*-glide planes perpendicular to [100], *a*-glide planes perpendicular to [010] and *n*-glide planes perpendicular to [001].

† Here we refer to the short or full Hermann–Mauguin symbol; the extended Hermann–Mauguin symbol, which is used much less often, does show all the symmetry elements (see Aroyo, 2016; Nespolo & Aroyo, 2016).

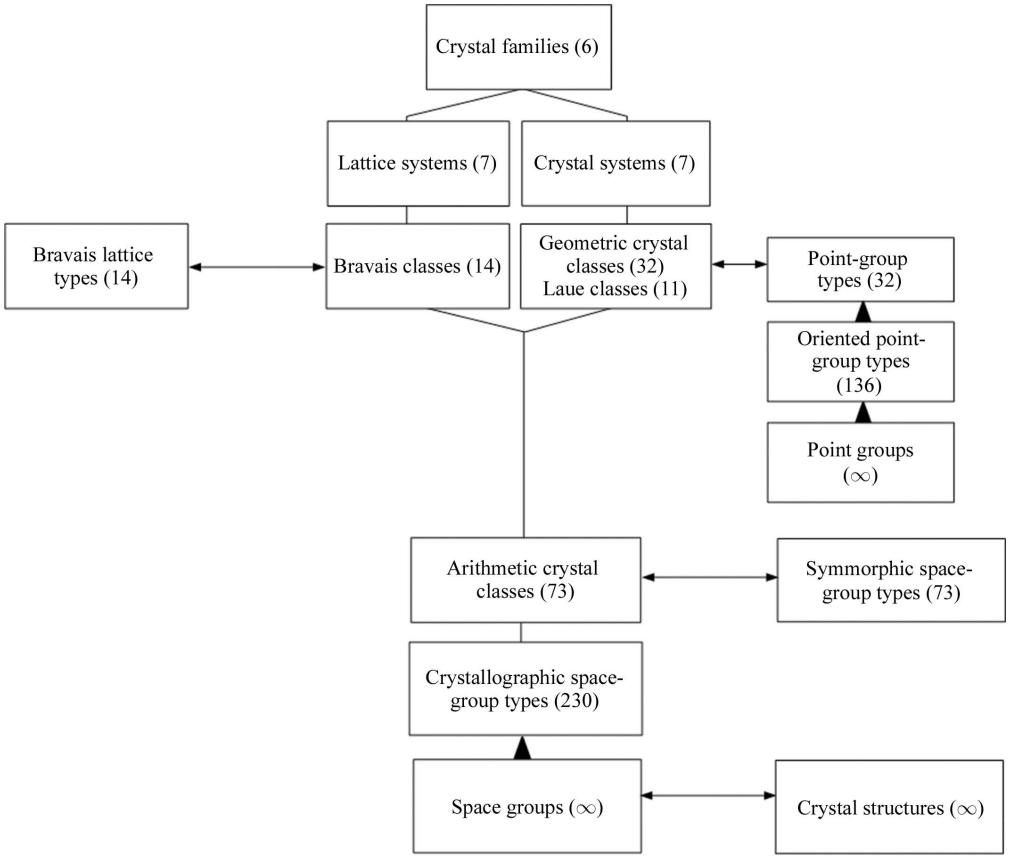


Figure 6
Hierarchy of the classification of space groups and point groups into classes, systems and families. Horizontal double-ended arrows indicate a 1:1 correspondence. Black triangles indicate that, in going from groups to types of groups, we do not consider cell parameters and the chosen coordinate system.

system' is incorrect, despite its widespread use in the French literature, where, for example, α-quartz is described as 'rhombohedral', despite the fact that the lattice is hexagonal. This confusion has a historical origin. In the XIX century, German and French crystallographers used the same term 'crystal system' (Kristallsystem; système cristallin) to indicate, respectively, what are today known as *crystal system* and *lattice system*.

Fig. 6 shows the full hierarchy of the classification of space groups discussed throughout this article, with the crystal families as the highest level.

10. Conclusion

We hope that the explanation and illustration of the various classification criteria for space groups given in this article will help others to apply these concepts correctly and will contribute to reducing misunderstandings due to imprecise terminology. As a quick reference to the reader, we have summarized in Table 4 common errors and why and how they should be corrected.

Acknowledgements

Critical remarks by two anonymous reviewers are gratefully acknowledged for their usefulness in improving the clarity of this article. MIA acknowledges the hospitality and support of CNRS-Nancy.

Funding information

The work of MIA was supported by the Government of the Basque Country (project No. IT779-13) and the Spanish Ministry of Economy and Competitiveness and FEDER funds (project No. MAT2015-66441-P).

References

Aroyo, M. I. (2016). Editor. *International Tables for Crystallography*, Vol. A, *Space-Group Symmetry*. Chichester: Wiley.
Aroyo, M. I. & Wondratschek, H. (1995). *Z. Kristallogr.* **210**, 243–254.
Flack, H. D. (2003). *Helv. Chim. Acta*, **86**, 905–921.
Flack, H. D, Wondratschek, H., Hahn, Th. & Abrahams, S. C. (2000). *Acta Cryst.* A**56**, 96–98.
Janner, A. (2004*a*). *Acta Cryst.* A**60**, 198–200.
Janner, A. (2004*b*). *Acta Cryst.* A**60**, 611–620.
Koch, E. & Fischer, W. (2006). *Z. Kristallogr.* **221**, 1–14.
Mumme, W. G. (1970). *Am. Mineral.* **55**, 367–377.
Nespolo, M. (2015*a*). *Cryst. Res. Technol.* **50**, 362–371.
Nespolo, M. (2015*b*). *J. Appl. Cryst.* **48**, 1290–1298.
Nespolo, M. (2017). *Cryst. Res. Technol.* **52**, 1600129.
Nespolo, M. & Aroyo, M. I. (2016). *Acta Cryst.* A**72**, 523–538.
Nespolo, M. & Ferraris, G. (2000). *Z. Kristallogr.* **215**, 77–81.
Nespolo, M. & Souvignier, B. (2009). *Z. Kristallogr.* **224**, 127–136.
Prewitt, C. T. & Burnham, C. W. (1966). *Am. Mineral.* **51**, 956–975.
Shuvalov, L. A. (1988). *Modern Crystallography IV. Physical Properties of Crystals*. Berlin: Springer.
Wintgen, G. (1941). *Math. Ann.* **118**, 195–215.
Wolff, P. M. de, Billiet, Y., Donnay, J. D. H., Fischer, W., Galiulin, R. B., Glazer, A. M., Hahn, Th., Senechal, M., Shoemaker, D. P., Wondratschek, H., Wilson, A. J. C. & Abrahams, S. C. (1992). *Acta Cryst.* A**48**, 727–732.
Wolff, P. M. de, Billiet, Y., Donnay, J. D. H., Fischer, W., Galiulin, R. B., Glazer, A. M., Senechal, M., Shoemaker, D. P., Wondratschek, H., Hahn, Th., Wilson, A. J. C. & Abrahams, S. C. (1989). *Acta Cryst.* A**45**, 494–499.