International Tables for Crystallography (2016). Vol. A, Section 1.3.4, pp. 31–41.

excluding 1. In particular, if the translation part of a coset representative is a lattice vector, it is usually chosen as the zero vector $\boldsymbol{o}$.

Note that due to the fact that $\mathcal{T}$ is a normal subgroup of $\mathcal{G}$, a system of coset representatives for the right cosets is at the same time a system of coset representatives for the left cosets.

1.3.3.3. Symmorphic and non-symmorphic space groups

If a coset with respect to the translation subgroup contains an operation of the form $(\boldsymbol{W}, \boldsymbol{w})$ with $\boldsymbol{w}$ a vector in the translation lattice, it is clear that the same coset also contains the operation $(\boldsymbol{W}, \boldsymbol{o})$ with trivial translation part. On the other hand, if a coset does not contain an operation of the form $(\boldsymbol{W}, \boldsymbol{o})$, this may be caused by an inappropriate choice of origin. For example, the operation $(-\boldsymbol{I}, (1/2, 1/2, 1/2))$ is turned into the inversion $(-\boldsymbol{I}, (0, 0, 0))$ by moving the origin to 1/4, 1/4, 1/4 (*cf.* Section 1.5.1.1 for a detailed treatment of origin-shift transformations).

Depending on the actual space group $\mathcal{G}$, it may or may not be possible to choose the origin such that every coset with respect to $\mathcal{T}$ contains an operation of the form $(\boldsymbol{W}, \boldsymbol{o})$.

Definition

Let $\mathcal{G}$ be a space group with translation subgroup $\mathcal{T}$. If it is possible to choose the coordinate system such that every coset of $\mathcal{G}$ with respect to $\mathcal{T}$ contains an operation $(\boldsymbol{W}, \boldsymbol{o})$ with trivial translation part, $\mathcal{G}$ is called a *symmorphic* space group, otherwise $\mathcal{G}$ is called a *non-symmorphic* space group.

One sees that the operations with trivial translation part form a subgroup of $\mathcal{G}$ which is isomorphic to a subgroup of the point group $\mathcal{P}$. This subgroup is the group of operations in $\mathcal{G}$ that fix the origin and is called the *site-symmetry group* of the origin (site-symmetry groups are discussed in detail in Section 1.4.4). It is the distinctive property of symmorphic space groups that they contain a subgroup which is isomorphic to the full point group. This may in fact be seen as an alternative definition for symmorphic space groups.

Proposition. A space group $\mathcal{G}$ with point group $\mathcal{P}$ is symmorphic if and only if it contains a subgroup isomorphic to $\mathcal{P}$. For a non-symmorphic space group $\mathcal{G}$, every finite subgroup of $\mathcal{G}$ is isomorphic to a proper subgroup of the point group.

Note that every finite subgroup of a space group is a subgroup of the site-symmetry group for some point, because finite groups cannot contain translations. Therefore, a symmorphic space group is characterized by the fact that it contains a site-symmetry group isomorphic to its point group, whereas in non-symmorphic space groups all site-symmetry groups have orders strictly smaller than the order of the point group.

Symmorphic space groups can easily be constructed by choosing a lattice $\mathbf{L}$ and a point group $\mathcal{P}$ which acts on $\mathbf{L}$. Then $\mathcal{G} = \{(\boldsymbol{W}, \boldsymbol{w}) \mid \boldsymbol{W} \in \mathcal{P}, \boldsymbol{w} \in \mathbf{L}\}$ is a space group in which the coset representatives can be chosen as $(\boldsymbol{W}, \boldsymbol{o})$.

Non-symmorphic space groups can also be constructed from a lattice $\mathbf{L}$ and a point group $\mathcal{P}$. What is required is a system of coset representatives with respect to $\mathcal{T}$ and these are obtained by choosing for each operation $\boldsymbol{W} \in \mathcal{P}$ a translation part $\boldsymbol{w}$. Owing to the translations, it is sufficient to consider vectors $\boldsymbol{w}$ with components between 0 and 1. However, the translation parts cannot be chosen arbitrarily, because for a point-group operation of order k, the operation $(\boldsymbol{W}, \boldsymbol{w})^k$ has to be a translation $(\boldsymbol{I}, \boldsymbol{t})$ with $\boldsymbol{t} \in \mathbf{L}$. Working this out, this imposes the restriction that

$$(\boldsymbol{W}^{k-1} + \ldots + \boldsymbol{W} + \boldsymbol{I})\boldsymbol{w} \in \mathbf{L}.$$

Once translation parts $\boldsymbol{w}$ are found that fulfil all these restrictions, one finally has to check whether the space group obtained this way is (by accident) symmorphic, but written with respect to an inappropriate origin. A change of origin by $\boldsymbol{p}$ is realized by conjugating the matrix–column pair $(\boldsymbol{W}, \boldsymbol{w})$ by the translation $(\boldsymbol{I}, -\boldsymbol{p})$ (*cf.* Section 1.5.1 on transformations of the coordinate system) which gives

$$(\boldsymbol{I}, -\boldsymbol{p})(\boldsymbol{W}, \boldsymbol{w})(\boldsymbol{I}, \boldsymbol{p}) = (\boldsymbol{W}, \boldsymbol{W}\boldsymbol{p} + \boldsymbol{w} - \boldsymbol{p}) = (\boldsymbol{W}, \boldsymbol{w} + (\boldsymbol{W} - \boldsymbol{I})\boldsymbol{p}).$$

Thus, the space group just constructed is symmorphic if there is a vector $\boldsymbol{p}$ such that $(\boldsymbol{W} - \boldsymbol{I})\boldsymbol{p} + \boldsymbol{w} \in \mathbf{L}$ for each of the coset representatives $(\boldsymbol{W}, \boldsymbol{w})$.

The above considerations also show how every space group can be assigned to a symmorphic space group in a canonical way, namely by setting the translation parts of coset representatives with respect to $\mathcal{T}$ to $\boldsymbol{o}$. This has the effect that screw rotations are turned into rotations and glide reflections into reflections. The Hermann–Mauguin symbol (see Section 1.4.1 for a detailed discussion of Hermann–Mauguin symbols) of the symmorphic space group to which an arbitrary space group is assigned is simply obtained by replacing any screw rotation symbol N_m by the corresponding rotation symbol N and every glide reflection symbol *a*, *b*, *c*, *d*, *e*, *n* by the symbol *m* for a reflection. A space group is found to be symmorphic if no such replacement is required, *i.e.* if the Hermann–Mauguin symbol 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.

Example

The space groups with Hermann-Mauguin symbols $P4mm$, $P4bm$, $P4_2cm$, $P4_2nm$, $P4cc$, $P4nc$, $P4_2mc$, $P4_2bc$ are all assigned to the symmorphic space group with Hermann–Mauguin symbol $P4mm$.

1.3.4. Classification of space groups

In this section we will consider various ways in which space groups may be grouped together. For the space groups themselves, the natural notion of equivalence is the classification into *space-group types*, but the point groups and lattices from which the space groups are built also have their own classification schemes into *geometric crystal classes* and *Bravais types of lattices*, respectively.

Some other types of classifications are relevant for certain applications, and these will also be considered. The hierarchy of the different classification levels and the numbers of classes on the different levels in dimension 3 are displayed in Fig. 1.3.4.1.

1.3.4.1. Space-group types

The main motivation behind studying space groups is that they allow the classification of crystal structures according to their symmetry properties. Since many properties of a structure can be derived from its group of symmetries alone, this allows the investigation of the properties of many structures simultaneously.

On the other hand, even for the same crystal structure the corresponding space group may look different, depending on the chosen coordinate system (see Chapter 1.5 for a detailed discussion of transformations to different coordinate systems). Because it is natural to regard two realizations of a group of symmetry operations with respect to two different coordinate systems as equivalent, the following notion of equivalence between space groups is natural.

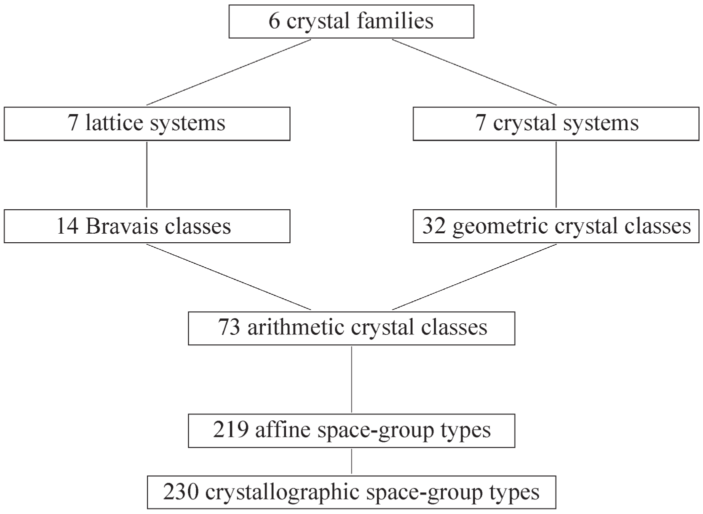

Figure 1.3.4.1
Classification levels for three-dimensional space groups.

Definition

Two space groups $\mathcal{G}$ and $\mathcal{G}'$ are called *affinely equivalent* if $\mathcal{G}'$ can be obtained from $\mathcal{G}$ by a change of the coordinate system. In terms of matrix–column pairs this means that there must exist a matrix–column pair $(\boldsymbol{P}, \boldsymbol{p})$ such that

$$\mathcal{G}' = \{(\boldsymbol{P}, \boldsymbol{p})^{-1}(\boldsymbol{W}, \boldsymbol{w})(\boldsymbol{P}, \boldsymbol{p}) \mid (\boldsymbol{W}, \boldsymbol{w}) \in \mathcal{G}\}.$$

The collection of space groups that are affinely equivalent with $\mathcal{G}$ forms the *affine type* of $\mathcal{G}$.

In dimension 2 there are 17 affine types of plane groups and in dimension 3 there are 219 affine space-group types. Note that in order to avoid misunderstandings we refrain from calling the space-group types *affine classes*, since the term classes is usually associated with *geometric crystal classes* (see below).

Grouping together space groups according to their space-group type serves different purposes. On the one hand, it is sometimes convenient to consider the same crystal structure and thus also its space group with respect to different coordinate systems, *e.g.* when the origin can be chosen in different natural ways or when a phase transition to a higher- or lower-symmetry phase with a different conventional cell is described. On the other hand, different crystal structures may give rise to the same space group once suitable coordinate systems have been chosen for both. We illustrate both of these perspectives by an example.

Examples

(i) The space group $\mathcal{G}$ of type $Pban$ (50) has a subgroup $\mathcal{H}$ of index 2 for which the coset representatives relative to the translation subgroup are the identity e: x, y, z, the twofold rotation g: $-x, y, -z$, the n glide h: $x+\frac{1}{2}, y+\frac{1}{2}, -z$ and the b glide k: $-x+\frac{1}{2}, y+\frac{1}{2}, z$. This subgroup is of type $Pb2n$, which is a non-conventional setting for $Pnc2$ (30). In the conventional setting, the coset representatives of $Pnc2$ are given by g': $-x, -y, z$, h': $-x, y+\frac{1}{2}, z+\frac{1}{2}$ and k': $x, -y+\frac{1}{2}, z+\frac{1}{2}$, *i.e.* with the z axis as rotation axis for the twofold rotation. The subgroup $\mathcal{H}$ can be transformed to its conventional setting by the basis transformation $(\mathbf{a}', \mathbf{b}', \mathbf{c}') = (\mathbf{c}, \mathbf{a}, \mathbf{b})$. Depending on whether the perspective of the full group $\mathcal{G}$ or the subgroup $\mathcal{H}$ is more important for a crystal structure, the groups $\mathcal{G}$ and $\mathcal{H}$ will be considered either with respect to the basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$ (conventional for $\mathcal{G}$) or to the basis $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ (conventional for $\mathcal{H}$).

(ii) The elements carbon, silicon and germanium all crystallize in the *diamond structure*, which has a face-centred cubic unit cell with two atoms shifted by 1/4 along the space diagonal of the conventional cubic cell. The space group is in all cases of type $Fd\bar{3}m$ (227), but the cell parameters differ: $a_{\rm C}$ = 3.5668 Å for carbon, $a_{\rm Si}$ = 5.4310 Å for silicon and $a_{\rm Ge}$ = 5.6579 Å for germanium (measured at 298 K). In order to scale the conventional cell of carbon to that of silicon, the coordinate system has to be transformed by the diagonal matrix

$$a_{\rm Si}/a_{\rm C} \cdot \boldsymbol{I}_3 \approx \begin{pmatrix} 1.523 & 0 & 0 \\ 0 & 1.523 & 0 \\ 0 & 0 & 1.523 \end{pmatrix}.$$

By a famous theorem of Bieberbach (see Bieberbach, 1911, 1912), affine equivalence of space groups actually coincides with the notion of abstract group isomorphism as discussed in Section 1.1.6.

Bieberbach theorem

Two space groups in n-dimensional space are isomorphic if and only if they are conjugate by an affine mapping.

This theorem is by no means obvious. Recall that for point groups the situation is very different, since for example the abstract cyclic group of order 2 is realized in the point groups of space groups of type $P2$, Pm and $P\bar{1}$, generated by a twofold rotation, reflection and inversion, respectively, which are clearly not equivalent in any geometric sense. The driving force behind the Bieberbach theorem is the special structure of space groups having an infinite normal translation subgroup on which the point group acts.

In crystallography, a notion of equivalence slightly stronger than affine equivalence is usually used. Since crystals occur in physical space and physical space can only be transformed by orientation-preserving mappings, space groups are only regarded as equivalent if they are conjugate by an *orientation-preserving* coordinate transformation, *i.e.* by an affine mapping that has a linear part with positive determinant.

Definition

Two space groups $\mathcal{G}$ and $\mathcal{G}'$ are said to belong to the same *space-group type* if $\mathcal{G}'$ can be obtained from $\mathcal{G}$ by an orientation-preserving coordinate transformation, *i.e.* by conjugation with a matrix–column pair $(\boldsymbol{P}, \boldsymbol{p})$ with $\det \boldsymbol{P} > 0$. In order to distinguish the space-group types explicitly from the affine space-group types (corresponding to the isomorphism classes), they are often called *crystallographic space-group types*.

The (crystallographic) space-group type collects together the infinitely many space groups that are obtained by expressing a single space group with respect to all possible right-handed coordinate systems for the point space.

Example

We consider the space group $\mathcal{G}$ of type $I4_1$ (80) which is generated by the right-handed fourfold screw rotation g: $-y, x+1/2, z+1/4$ (located at $-1/4, 1/4, z$), the centring translation t: $x+1/2, y+1/2, z+1/2$ and the integral translations of a primitive tetragonal lattice. Conjugating the group $\mathcal{G}$ to $\mathcal{G}' = m\mathcal{G}m^{-1}$ by the reflection m in the plane $z = 0$ turns the right-handed screw rotation g into the left-handed screw

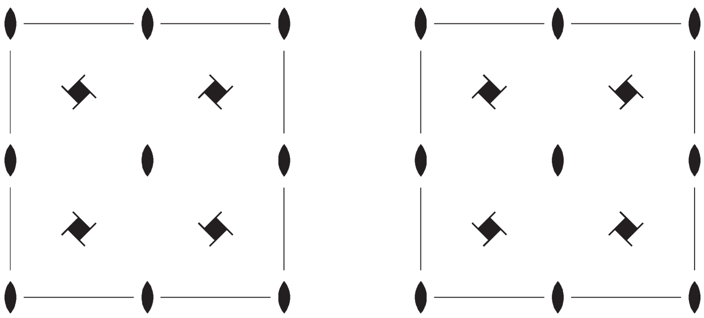

Figure 1.3.4.2
Space-group diagram of $I4_1$ (left) and its reflection in the plane $z = 0$ (right).

rotation g': $-y, x+1/2, z-1/4$, and one might suspect that $\mathcal{G}'$ is a space group of the same affine type but of a different crystallographic space-group type as $\mathcal{G}$. However, this is not the case because conjugating $\mathcal{G}$ by the translation $n = t(0, 1/2, 0)$ conjugates g to $g'' = ngn^{-1}$: $-y+1/2, x+1, z+1/4$. One sees that g'' is the composition of g' with the centring translation t and hence g'' belongs to $\mathcal{G}'$. This shows that conjugating $\mathcal{G}$ by either the reflection m or the translation n both result in the same group $\mathcal{G}'$. This can also be concluded directly from the space-group diagrams in Fig. 1.3.4.2. Reflecting in the plane $z = 0$ turns the diagram on the left into the diagram on the right, but the same effect is obtained when the left diagram is shifted by $\frac{1}{2}$ along either **a** or **b**.

The groups $\mathcal{G}$ and $\mathcal{G}'$ thus belong to the same crystallographic space-group type because $\mathcal{G}$ is transformed to $\mathcal{G}'$ by a shift of the origin by $\frac{1}{2}\mathbf{b}$, which is clearly an orientation-preserving coordinate transformation.

Enantiomorphism

The 219 affine space-group types in dimension 3 result in 230 crystallographic space-group types. Since an affine type either forms a single space-group type (in the case where the group obtained by an orientation-reversing coordinate transformation can also be obtained by an orientation-preserving transformation) or splits into two space-group types, this means that there are 11 affine space-group types such that an orientation-reversing coordinate transformation cannot be compensated by an orientation-preserving transformation.

Groups that differ only by their handedness are closely related to each other and share many properties. One addresses this phenomenon by the concept of *enantiomorphism*.

Example

Let $\mathcal{G}$ be a space group of type $P4_1$ (76) generated by a fourfold right-handed screw rotation $(4^+_{001}, (0,0,1/4))$ and the translations of a primitive tetragonal lattice. Then transforming the coordinate system by a reflection in the plane $z = 0$ results in a space group $\mathcal{G}'$ with fourfold left-handed screw rotation $(4^-_{001}, (0,0,1/4)) = (4^+_{001}, (0,0,-1/4))^{-1}$. The groups $\mathcal{G}$ and $\mathcal{G}'$ are isomorphic because they are conjugate by an affine mapping, but $\mathcal{G}'$ belongs to a different space-group type, namely $P4_3$ (78), because $\mathcal{G}$ does not contain a fourfold left-handed screw rotation with translation part $\frac{1}{4}\mathbf{c}$.

Definition

Two space groups $\mathcal{G}$ and $\mathcal{G}'$ are said to form an *enantiomorphic pair* if they are conjugate under an affine mapping, but not under an orientation-preserving affine mapping.

If $\mathcal{G}$ is the group of isometries of some crystal pattern, then its enantiomorphic counterpart $\mathcal{G}'$ is the group of isometries of the mirror image of this crystal pattern.

The splitting of affine space-group types of three-dimensional space groups into pairs of crystallographic space-group types gives rise to the following 11 enantiomorphic pairs of space-group types: $P4_1/P4_3$ (76/78), $P4_122/P4_322$ (91/95), $P4_12_12/P4_32_12$ (92/96), $P3_1/P3_2$ (144/145), $P3_112/P3_212$ (151/153), $P3_121/P3_221$ (152/154), $P6_1/P6_5$ (169/173), $P6_2/P6_4$ (170/172), $P6_122/P6_522$ (178/179), $P6_222/P6_422$ (180/181), $P4_332/P4_132$ (212/213). These groups are easily recognized by their Hermann–Mauguin symbols, because they are the primitive groups for which the Hermann–Mauguin symbol contains one of the screw rotations 3_1, 3_2, 4_1, 4_3, 6_1, 6_2, 6_4 or 6_5. The groups with fourfold screw rotations and body-centred lattices do not give rise to enantiomorphic pairs, because in these groups the orientation reversal can be compensated by an origin shift, as illustrated in the example above for the group of type $I4_1$.

Example

A well known example of a crystal that occurs in forms whose symmetry is described by enantiomorphic pairs of space groups is quartz. For low-temperature α-quartz there exists a left-handed and a right-handed form with space groups $P3_121$ (152) and $P3_221$ (154), respectively. The two individuals of opposite chirality occur together in the so-called Brazil twin of quartz. At higher temperatures, a phase transition leads to the higher-symmetry β-quartz forms, with space groups $P6_422$ (181) and $P6_222$ (180), which still form an enantiomorphic pair.

1.3.4.2. Geometric crystal classes

We recall that the point group of a space group is the group of linear parts occurring in the space group. Once a basis for the underlying vector space is chosen, such a point group is a group of 3×3 matrices. A point group is characterized by the relative positions between the rotation and rotoinversion axes and the reflection planes of the operations it contains, and in this sense a point group is independent of the chosen basis. However, a suitable choice of basis is useful to highlight the geometric properties of a point group.

Example

A point group of type $3m$ is generated by a threefold rotation and a reflection in a plane with normal vector perpendicular to the rotation axis. Choosing a basis **a**, **b**, **c** such that **c** is along the rotation axis, **a** is perpendicular to the reflection plane and **b** is the image of **a** under the threefold rotation (*i.e.* **b** lies in the plane perpendicular to the rotation axis and makes an angle of 120° with **a**), the matrices of the threefold rotation and the reflection with respect to this basis are

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

A different useful basis is obtained by choosing a vector $\mathbf{a}'$ in the reflection plane but neither along the rotation axis nor perpendicular to it and taking $\mathbf{b}'$ and $\mathbf{c}'$ to be the images of $\mathbf{a}'$ under the threefold rotation and its square. Then the matrices of the threefold rotation and the reflection with respect to the basis $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$ are

$$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \text{ and } \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}.$$

Different choices of a basis for a point group in general result in different matrix groups, and it is natural to consider two point groups as equivalent if they are transformed into each other by a basis transformation. This is entirely analogous to the situation of space groups, where space groups that only differ by the choice of coordinate system are regarded as equivalent. This notion of equivalence is applied at both the level of space groups and point groups.

Definition

Two space groups $\mathcal{G}$ and $\mathcal{G}'$ with point groups $\mathcal{P}$ and $\mathcal{P}'$, respectively, are said to belong to the same *geometric crystal class* if $\mathcal{P}$ and $\mathcal{P}'$ become the same matrix group once suitable bases for the three-dimensional space are chosen.

Equivalently, $\mathcal{G}$ and $\mathcal{G}'$ belong to the same geometric crystal class if the point group $\mathcal{P}'$ can be obtained from $\mathcal{P}$ by a basis transformation of the underlying vector space $\mathbb{V}^3$, *i.e.* if there is an invertible 3×3 matrix $\boldsymbol{P}$ such that

$$\mathcal{P}' = \{\boldsymbol{P}^{-1}\boldsymbol{W}\boldsymbol{P} \mid \boldsymbol{W} \in \mathcal{P}\}.$$

Also, two matrix groups $\mathcal{P}$ and $\mathcal{P}'$ are said to belong to the same geometric crystal class if they are conjugate by an invertible 3×3 matrix $\boldsymbol{P}$.

Historically, the geometric crystal classes in dimension 3 were determined much earlier than the space groups. They were obtained as the symmetry groups for the set of normal vectors of crystal faces which describe the morphological symmetry of crystals.

Note that for the geometric crystal classes in dimension 3 (and in all other odd dimensions) the distinction between orientation-preserving and orientation-reversing transformations is irrelevant, since any conjugation by an arbitrary transformation can already be realized by an orientation-preserving transformation. This is due to the fact that the inversion $-\boldsymbol{I}$ on the one hand commutes with every matrix $\boldsymbol{W}$, *i.e.* $(-\boldsymbol{I})\boldsymbol{W} = \boldsymbol{W}(-\boldsymbol{I})$, and on the other hand $\det(-\boldsymbol{I}) = -1$. If $\boldsymbol{P}$ is orientation reversing, one has $\det \boldsymbol{P} < 0$ and then $(-\boldsymbol{I})\boldsymbol{P} = -\boldsymbol{P}$ is orientation preserving because $\det(-\boldsymbol{P}) = -\det \boldsymbol{P} > 0$. But $(-\boldsymbol{P})^{-1}\boldsymbol{W}(-\boldsymbol{P}) = \boldsymbol{P}^{-1}\boldsymbol{W}\boldsymbol{P}$, hence the transformations by $\boldsymbol{P}$ and $-\boldsymbol{P}$ give the same result and one of $\boldsymbol{P}$ and $-\boldsymbol{P}$ is orientation preserving.

Remark: One often speaks of the geometric crystal classes as the *types of point groups*. This emphasizes the point of view in which a point group is regarded as the group of linear parts of a space group, written with respect to an *arbitrary basis* of $\mathbb{R}^n$ (not necessarily a lattice basis).

It is also common to state that *there are 32 point groups in three-dimensional space*. This is just as imprecise as saying that *there are 230 space groups*, since there are in fact infinitely many point groups and space groups.

What is meant when we say that two space groups have *the same point group* is usually that their point groups are of the same type (*i.e.* lie in the same geometric crystal class) and can thus be *made to coincide* by a suitable basis transformation.

Example

In the space group $P3$ the threefold rotation generating the point group is given by the matrix

$$\boldsymbol{W} = \begin{pmatrix} 0 & -1 & 0 \\ 1 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

whereas in the space group $R3$ (in the rhombohedral setting) the threefold rotation is given by the matrix

$$\boldsymbol{W}' = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}.$$

These two matrices are conjugate by the basis transformation

$$\boldsymbol{P} = \frac{1}{3}\begin{pmatrix} 1 & 0 & -1 \\ 0 & 1 & -1 \\ 1 & 1 & 1 \end{pmatrix},$$

which transforms the basis of the hexagonal setting into that of the rhombohedral setting. This shows that the space groups $P3$ and $R3$ belong to the same geometric crystal class.

The example is typical in the sense that different groups in the same geometric crystal class usually describe the same group of linear parts acting on different lattices, *e.g.* primitive and centred. Writing the action of the linear parts with respect to primitive bases of different lattices gives rise to different matrix groups.

1.3.4.3. Bravais types of lattices and Bravais classes

In the classification of space groups into geometric crystal classes, only the point-group part is considered and the translation lattice is ignored. It is natural that the converse point of view is also adopted, where space groups are grouped together according to their translation lattices, irrespective of what the point groups are.

We have already seen that a lattice can be characterized by its metric tensor, containing the scalar products of a primitive basis. If a point group $\mathcal{P}$ acts on a lattice $\mathbf{L}$, it fixes the metric tensor $\boldsymbol{G}$ of $\mathbf{L}$, *i.e.* $\boldsymbol{W}^{\rm T} \cdot \boldsymbol{G} \cdot \boldsymbol{W} = \boldsymbol{G}$ for all $\boldsymbol{W}$ in $\mathcal{P}$ and is thus a subgroup of the Bravais group $Aut(\mathbf{L})$ of $\mathbf{L}$. Also, a matrix group $\mathcal{B}$ is called a *Bravais group* if it is the Bravais group $Aut(\mathbf{L})$ for some lattice $\mathbf{L}$. The Bravais groups govern the classification of lattices.

Definition

Two lattices $\mathbf{L}$ and $\mathbf{L}'$ belong to the same *Bravais type of lattices* if their Bravais groups $Aut(\mathbf{L})$ and $Aut(\mathbf{L}')$ are the same matrix group when written with respect to suitable primitive bases of $\mathbf{L}$ and $\mathbf{L}'$.

Note that in order to have the same Bravais group, the metric tensors of the two lattices $\mathbf{L}$ and $\mathbf{L}'$ do not have to be the same or scalings of each other.

Example

The mineral rutile (TiO_2) has a space group of type $P4_2/mnm$ (136) with a primitive tetragonal cell with cell parameters $a = b$ = 4.594 Å and c = 2.959 Å. The metric tensor of the translation lattice $\mathbf{L}$ is therefore

$$\boldsymbol{G} = \begin{pmatrix} 4.594^2 & 0 & 0 \\ 0 & 4.594^2 & 0 \\ 0 & 0 & 2.959^2 \end{pmatrix}$$

and the Bravais group of the lattice is generated by the fourfold rotation

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

around the z axis, the reflection

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

in the plane $x = 0$ and the reflection

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

in the plane $z = 0$.

The silicate mineral cristobalite also has (at low temperatures) a primitive tetragonal cell with $a = b = 4.971$ Å and $c = 6.928$ Å, and the space-group type is $P4_12_12$ (92). In this case the metric tensor of the translation lattice $\mathbf{L}'$ is

$$\boldsymbol{G}' = \begin{pmatrix} 4.971^2 & 0 & 0 \\ 0 & 4.971^2 & 0 \\ 0 & 0 & 6.928^2 \end{pmatrix}$$

and one checks that the Bravais group of $\mathbf{L}'$ is precisely the same as that of $\mathbf{L}$. Therefore, the translation lattices $\mathbf{L}$ for rutile and $\mathbf{L}'$ for cristobalite belong to the same Bravais type of lattices.

The different Bravais types of lattices, their cell parameters and metric tensors are displayed in Tables 3.1.2.1 (dimension 2) and 3.1.2.2 (dimension 3): in dimension 2 there are 5 Bravais types and in dimension 3 there are 14 Bravais types of lattices.

It is crucial for the classification of lattices *via* their Bravais groups that one works with primitive bases, because a primitive and a body-centred cubic lattice have the same automorphisms when written with respect to the conventional cubic basis, but are clearly different types of lattices.

Example

The silicate mineral zircon ($ZrSiO_4$) has a body-centred tetragonal cell with cell parameters $a = b = 6.607$ Å and $c = 5.982$ Å. The body-centred translation lattice $\mathbf{L}'$ is spanned by the primitive tetragonal lattice $\mathbf{L}$ with basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$ with $\alpha = \beta = \gamma = 90°$ and the centring vector $\mathbf{v} = \frac{1}{2}(\mathbf{a} + \mathbf{b} + \mathbf{c})$. A primitive basis of $\mathbf{L}'$ is obtained as $(\mathbf{a}', \mathbf{b}', \mathbf{c}') = (\mathbf{a}, \mathbf{b}, \mathbf{c})\boldsymbol{P}$ with

$$\boldsymbol{P} = \frac{1}{2}\begin{pmatrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{pmatrix},$$

i.e. $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b} + \mathbf{c}) = -\mathbf{a} + \mathbf{v}$, $\mathbf{b}' = \frac{1}{2}(\mathbf{a} - \mathbf{b} + \mathbf{c}) = -\mathbf{b} + \mathbf{v}$, $\mathbf{c}' = \frac{1}{2}(\mathbf{a} + \mathbf{b} - \mathbf{c}) = -\mathbf{c} + \mathbf{v}$ and the metric tensor $\boldsymbol{G}'$ of $\mathbf{L}'$ with respect to the primitive basis $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ is

$$\boldsymbol{G}' = \boldsymbol{P}^{\mathrm{T}}\begin{pmatrix} 6.607^2 & 0 & 0 \\ 0 & 6.607^2 & 0 \\ 0 & 0 & 5.982^2 \end{pmatrix}\boldsymbol{P} = \begin{pmatrix} 5.547^2 & -12.880 & -8.946 \\ -12.880 & 5.547^2 & -8.946 \\ -8.946 & -8.946 & 5.547^2 \end{pmatrix}.$$

The Bravais group of the primitive tetragonal lattice $\mathbf{L}$ is generated (as in the previous example) by

$$\boldsymbol{W}_1 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \boldsymbol{W}_2 = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$
$$\text{and } \boldsymbol{W}_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix},$$

and these matrices also generate the Bravais group of the body-centred tetragonal lattice $\mathbf{L}'$, but written with respect to the primitive basis $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ these matrices are transformed to

$$\boldsymbol{W}_1' = \boldsymbol{P}^{-1}\boldsymbol{W}_1\boldsymbol{P} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 1 & -1 \\ -1 & 1 & 0 \end{pmatrix},$$
$$\boldsymbol{W}_2' = \boldsymbol{P}^{-1}\boldsymbol{W}_2\boldsymbol{P} = \begin{pmatrix} 1 & 0 & 0 \\ 1 & 0 & -1 \\ 1 & -1 & 0 \end{pmatrix} \text{ and}$$
$$\boldsymbol{W}_3' = \boldsymbol{P}^{-1}\boldsymbol{W}_3\boldsymbol{P} = \begin{pmatrix} 0 & -1 & 1 \\ -1 & 0 & 1 \\ 0 & 0 & 1 \end{pmatrix}.$$

That the primitive and the body-centred tetragonal lattices have different types ultimately follows from the fact that the body-centred lattice $\mathbf{L}'$ does not have a primitive basis consisting of vectors $\mathbf{a}'', \mathbf{b}'', \mathbf{c}''$ which are pairwise perpendicular and such that $\mathbf{a}''$ and $\mathbf{b}''$ have the same length. This would be required to have the matrices $\boldsymbol{W}_1$, $\boldsymbol{W}_2$ and $\boldsymbol{W}_3$ in the Bravais group of $\mathbf{L}'$.

As we have seen, the metric tensors of lattices belonging to the same Bravais type need not be the same, but if they are written with respect to suitable bases they are found to have the same structure, differing only in the specific values for certain free parameters.

Definition

Let $\mathbf{L}$ be a lattice with metric tensor $\boldsymbol{G}$ with respect to a primitive basis and let $\mathcal{B} = Aut(\mathbf{L}) = \{\boldsymbol{W} \in \mathrm{GL}_3(\mathbb{Z}) \mid \boldsymbol{W}^{\mathrm{T}} \cdot \boldsymbol{G} \cdot \boldsymbol{W} = \boldsymbol{G}\}$ be the Bravais group of $\mathbf{L}$. Then

$$\mathbf{M}(\mathcal{B}) := \{\boldsymbol{G}' \text{ symmetric } 3 \times 3 \text{ matrix} \mid \boldsymbol{W}^{\mathrm{T}} \cdot \boldsymbol{G}' \cdot \boldsymbol{W} = \boldsymbol{G}' \text{ for all } \boldsymbol{W} \in \mathcal{B}\}$$

is called the *space of metric tensors* of $\mathcal{B}$. The dimension of $\mathbf{M}(\mathcal{B})$ is called the *number of free parameters* of the lattice $\mathbf{L}$. Analogously, for an arbitrary integral matrix group $\mathcal{P}$,

$$\mathbf{M}(\mathcal{P}) := \{\boldsymbol{G}' \text{ symmetric } 3 \times 3 \text{ matrix} \mid \boldsymbol{W}^{\mathrm{T}} \cdot \boldsymbol{G}' \cdot \boldsymbol{W} = \boldsymbol{G}' \text{ for all } \boldsymbol{W} \in \mathcal{P}\}$$

is called the *space of metric tensors* of $\mathcal{P}$. If $\dim \mathbf{M}(\mathcal{P}') = \dim \mathbf{M}(\mathcal{P})$ for a subgroup $\mathcal{P}'$ of $\mathcal{P}$, the spaces of metric tensors are the same for both groups and one says that $\mathcal{P}'$ *does not act on a more general lattice* than $\mathcal{P}$ does.

It is clear that $\mathbf{M}(\mathcal{B})$ contains in particular the metric tensor $\boldsymbol{G}$ of the lattice $\mathbf{L}$ of which $\mathcal{B}$ is the Bravais group. Moreover, $\mathcal{B}$ is a subgroup of the Bravais group of every lattice with metric tensor in $\mathbf{M}(\mathcal{B})$.

Example

Let $\mathbf{L}$ be a lattice with metric tensor

$$\begin{pmatrix} 17 & 0 & 0 \\ 0 & 17 & 0 \\ 0 & 0 & 42 \end{pmatrix},$$

then $\mathbf{L}$ is a tetragonal lattice with Bravais group $\mathcal{B}$ of type $4/mmm$ generated by the fourfold rotation

$$\boldsymbol{W}_1 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

and the reflections

$$\boldsymbol{W}_2 = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \text{ and } \boldsymbol{W}_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

The space of metric tensors of $\mathcal{B}$ is

$$\mathbf{M}(\mathcal{B}) = \left\{ \begin{pmatrix} g_{11} & 0 & 0 \\ 0 & g_{11} & 0 \\ 0 & 0 & g_{33} \end{pmatrix} \mid g_{11}, g_{33} \in \mathbb{R} \right\}$$

and the number of free parameters of $\mathbf{L}$ is 2.

For every lattice $\mathbf{L}'$ with metric tensor $\boldsymbol{G}'$ in $\mathbf{M}(\mathcal{B})$ such that $g_{11} \neq g_{33}$, one can check that the Bravais group of $\mathbf{L}'$ is equal to $\mathcal{B}$, hence these lattices belong to the same Bravais type of lattices as $\mathbf{L}$. On the other hand, if it happens that $g_{11} = g_{33}$ in the metric tensor $\boldsymbol{G}'$ of a lattice $\mathbf{L}'$, then the Bravais group of $\mathbf{L}'$ is the full cubic point group of type $m\bar{3}m$ and $\mathcal{B}$ is a proper subgroup of the Bravais group of $\mathbf{L}'$. In this case the lattice $\mathbf{L}'$ is of a different Bravais type to $\mathbf{L}$, namely cubic.

The subgroup $\mathcal{P}$ of $\mathcal{B}$ generated only by the fourfold rotation $\boldsymbol{W}_1$ has the same space of metric tensors as $\mathcal{B}$, thus this subgroup acts on the same types of lattices as $\mathcal{B}$ (*i.e.* tetragonal lattices). On the other hand, for the subgroup $\mathcal{P}'$ of $\mathcal{B}$ generated by the reflections $\boldsymbol{W}_2$ and $\boldsymbol{W}_3$, the space of metric tensors is

$$\mathbf{M}(\mathcal{P}') = \left\{ \begin{pmatrix} g_{11} & 0 & 0 \\ 0 & g_{22} & 0 \\ 0 & 0 & g_{33} \end{pmatrix} \mid g_{11}, g_{22}, g_{33} \in \mathbb{R} \right\}$$

and is thus of dimension 3. This shows that the subgroup $\mathcal{P}'$ acts on more general lattices than $\mathcal{B}$, namely on orthorhombic lattices.

Remark: The metric tensor of a lattice basis is a *positive definite*[2] matrix. It is clear that not all matrices in $\mathbf{M}(\mathcal{B})$ are positive definite [if $\boldsymbol{G} \in \mathbf{M}(\mathcal{B})$ is positive definite, then $-\boldsymbol{G}$ is certainly not positive definite], but the different geometries of lattices on which $\mathcal{B}$ acts are represented precisely by the positive definite metric tensors in $\mathbf{M}(\mathcal{B})$.

The space of metric tensors obtained from a lattice can be interpreted as an expression of the metric tensor with general entries, *i.e.* as a generic metric tensor describing the different lattices within the same Bravais type. Special choices for the entries may lead to lattices with accidental higher symmetry, which is in fact a common phenomenon in phase transitions caused by changes of temperature or pressure.

One says that the translation lattice $\mathbf{L}$ of a space group $\mathcal{G}$ with point group $\mathcal{P}$ has a *specialized metric* if the dimension of the space of metric tensors of $\mathcal{B} = Aut(\mathbf{L})$ is smaller than the dimension of the space of metric tensors of $\mathcal{P}$. Viewed from a slightly different angle, a specialized metric occurs if the location of the atoms within the unit cell reduces the symmetry of the translation lattice to that of a different lattice type.

Example

A space group $\mathcal{G}$ of type $P2/m$ (10) with cell parameters $a = 4.4$, $b = 5.5$, $c = 6.6$ Å, $\alpha = \beta = \gamma = 90°$ has a specialized metric, because the point group $\mathcal{P}$ of type $2/m$ is generated by

$$\boldsymbol{W} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

and $-\boldsymbol{I}$, and has

$$\mathbf{M}(\mathcal{P}) = \left\{ \begin{pmatrix} g_{11} & 0 & g_{13} \\ 0 & g_{22} & 0 \\ g_{13} & 0 & g_{33} \end{pmatrix} \mid g_{11}, g_{22}, g_{33}, g_{13} \in \mathbb{R} \right\}$$

as its space of metric tensors, which is of dimension 4. The lattice $\mathbf{L}$ with the given cell parameters, however, is orthorhombic, since the free parameter g_{13} is specialized to $g_{13} = 0$. The automorphism group $Aut(\mathbf{L})$ is of type mmm and has a space of metric tensors of dimension 3, namely

$$\left\{ \begin{pmatrix} g_{11} & 0 & 0 \\ 0 & g_{22} & 0 \\ 0 & 0 & g_{33} \end{pmatrix} \mid g_{11}, g_{22}, g_{33} \in \mathbb{R} \right\}.$$

The higher symmetry of the translation lattice would, for example, be destroyed by an atomic configuration compatible with the lattice and represented by only two atoms in the unit cell located at 0.17, 1/2, 0.42 and 0.83, 1/2, 0.58. The two atoms are related by a twofold rotation around the b axis, which indicates the invariance of the configuration under twofold rotations with axes parallel to $\mathbf{b}$, but in contrast to the lattice $\mathbf{L}$, the atomic configuration is not compatible with rotations around the a or the c axes.

By looking at the spaces of metric tensors, space groups can be classified according to the Bravais types of their translation lattices, without suffering from complications due to specialized metrics.

Definition

Let $\mathbf{L}$ be a lattice with metric tensor $\boldsymbol{G}$ and Bravais group $\mathcal{B} = Aut(\mathbf{L})$ and let $\mathbf{M}(\mathcal{B})$ be the space of metric tensors associated to $\mathbf{L}$. Then those space groups $\mathcal{G}$ form the *Bravais class* corresponding to the Bravais type of $\mathbf{L}$ for which $\mathbf{M}(\mathcal{P}) = \mathbf{M}(\mathcal{B})$ when the point group $\mathcal{P}$ of $\mathcal{G}$ is written with respect to a suitable primitive basis of the translation lattice of $\mathcal{G}$. The names for the Bravais classes are the same as those for the corresponding Bravais types of lattices.

The Bravais groups of lattices provide a link between lattices and point groups, the two building blocks of space groups. However, although the Bravais group of a lattice is simply a matrix group, the fact that it is expressed with respect to a primitive basis and fixes the metric tensor of the lattice preserves the necessary information about the lattice. When the Bravais group is regarded as a point group, the information about the lattice is lost, since point groups can be written with respect to an arbitrary basis. In order to distinguish Bravais groups of lattices at the level of point groups and geometric crystal classes, the concept of a holohedry is introduced.

[2] A symmetric matrix $\boldsymbol{G}$ is *positive definite* if $\mathbf{v}^{\mathrm{T}} \cdot \boldsymbol{G} \cdot \mathbf{v} > 0$ for every vector $\mathbf{v} \neq 0$.

Definition

The geometric crystal class of a point group $\mathcal{P}$ is called a *holohedry* (or *lattice point group*, *cf.* Chapters 3.1 and 3.3) if $\mathcal{P}$ is the Bravais group of some lattice $\mathbf{L}$.

Example

Let $\mathcal{P}$ be the point group of type $\bar{3}m$ generated by the threefold rotoinversion

$$\boldsymbol{W}_1 = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

around the z axis and the twofold rotation

$$\boldsymbol{W}_2 = \begin{pmatrix} 1 & -1 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix},$$

expressed with respect to the conventional basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$ of a hexagonal lattice. The group $\mathcal{P}$ is not the Bravais group of the lattice $\mathbf{L}$ spanned by $\mathbf{a}, \mathbf{b}, \mathbf{c}$ because this lattice also allows a sixfold rotation around the z axis, which is not contained in $\mathcal{P}$. But $\mathcal{P}$ also acts on the rhombohedrally centred lattice $\mathbf{L}'$ with primitive basis $\mathbf{a}' = \frac{1}{3}(2\mathbf{a} + \mathbf{b} + \mathbf{c})$, $\mathbf{b}' = \frac{1}{3}(-\mathbf{a} + \mathbf{b} + \mathbf{c})$, $\mathbf{c}' = \frac{1}{3}(-\mathbf{a} - 2\mathbf{b} + \mathbf{c})$. With respect to the basis $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ the rotoinversion and twofold rotation are transformed to

$$\boldsymbol{W}'_1 = \begin{pmatrix} 0 & 0 & -1 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix} \text{ and } \boldsymbol{W}'_2 = \begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix},$$

and these matrices indeed generate the Bravais group of $\mathbf{L}'$. The geometric crystal class with symbol $\bar{3}m$ is therefore a holohedry.

Note that in dimension 3 the above is actually the only example of a geometric crystal class in which the point groups are Bravais groups for some but not for all the lattices on which they act. In all other cases, each matrix group $\mathcal{P}$ corresponding to a holohedry is actually the Bravais group of the lattice spanned by the basis with respect to which $\mathcal{P}$ is written.

1.3.4.4. Other classifications of space groups

In this section we summarize a number of other classification schemes which are perhaps of slightly lower significance than those of space-group types, geometric crystal classes and Bravais types of lattices, but also play an important role for certain applications.

1.3.4.4.1. Arithmetic crystal classes

We have already seen that every space group can be assigned to a symmorphic space group in a natural way by setting the translation parts of coset representatives with respect to the translation subgroup to $\boldsymbol{o}$. The groups assigned to a symmorphic space group in this way all have the same translation lattice and the same point group but the different possibilities for the interplay between these two parts are ignored.

If we want to collect together all space groups that correspond to symmorphic space groups of the same type, we arrive at the classification into *arithmetic crystal classes*. This can also be seen as a classification of the symmorphic space-group types. The distribution of the space groups into arithmetic classes, represented by the corresponding symmorphic space-group types, is given in Table 2.1.3.3.

The crucial observation for characterizing this classification is that space groups that correspond to the same symmorphic space group all have translation lattices of the same Bravais type. This means that the freedom in the choice of a basis transformation of the underlying vector space is restricted, because a primitive basis has to be mapped again to a primitive basis. Assuming that the point groups are written with respect to primitive bases, this means that the basis transformation is an integral matrix with determinant ± 1.

Definition

Two space groups $\mathcal{G}$ and $\mathcal{G}'$ with point groups $\mathcal{P}$ and $\mathcal{P}'$, respectively, both written with respect to primitive bases of their translation lattices, are said to lie in the same *arithmetic crystal class* if $\mathcal{P}'$ can be obtained from $\mathcal{P}$ by an integral basis transformation of determinant ± 1, *i.e.* if there is an integral 3×3 matrix $\boldsymbol{P}$ with $\det \boldsymbol{P} = \pm 1$ such that

$$\mathcal{P}' = \{\boldsymbol{P}^{-1}\boldsymbol{W}\boldsymbol{P} \mid \boldsymbol{W} \in \mathcal{P}\}.$$

Also, two integral matrix groups $\mathcal{P}$ and $\mathcal{P}'$ are said to belong to the same arithmetic crystal class if they are conjugate by an integral 3×3 matrix $\boldsymbol{P}$ with $\det \boldsymbol{P} = \pm 1$.

Example

Let

$$\boldsymbol{M}_1 = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \boldsymbol{M}_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$
$$\text{and } \boldsymbol{M}_3 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

be reflections in the planes $x = 0$, $y = 0$ and $x = y$, respectively, and let $\mathcal{P}_1 = \langle \boldsymbol{M}_1 \rangle$, $\mathcal{P}_2 = \langle \boldsymbol{M}_2 \rangle$ and $\mathcal{P}_3 = \langle \boldsymbol{M}_3 \rangle$ be the integral matrix groups generated by these reflections. Then $\mathcal{P}_1$ and $\mathcal{P}_2$ belong to the same arithmetic crystal class because they are transformed into each other by the basis transformation

$$\boldsymbol{P} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

interchanging the x and y axes. But $\mathcal{P}_3$ belongs to a different arithmetic crystal class, because $\boldsymbol{M}_3$ is not conjugate to $\boldsymbol{M}_1$ by an integral matrix $\boldsymbol{P}$ of determinant ± 1. The two groups $\mathcal{P}_1$ and $\mathcal{P}_3$ belong, however, to the same geometric crystal class, because $\boldsymbol{M}_1$ and $\boldsymbol{M}_3$ are transformed into each other by the basis transformation

$$\boldsymbol{P} = \begin{pmatrix} \frac{1}{2} & -\frac{1}{2} & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

which has determinant $\frac{1}{2}$. This basis transformation shows that $\boldsymbol{M}_1$ and $\boldsymbol{M}_3$ can be interpreted as the action of the same reflection on a primitive lattice and on a C-centred lattice.

As explained above, the number of arithmetic crystal classes is equal to the number of symmorphic space-group types: in dimension 2 there are 13 such classes, in dimension 3 there are 73 arithmetic crystal classes. The Hermann–Mauguin symbol of the symmorphic space-group type to which a space group $\mathcal{G}$ belongs is obtained from the symbol for the space-group type of $\mathcal{G}$ by replacing any screw-rotation axis symbol N_m by the corresponding rotation axis symbol N and every glide-plane symbol a, b, c, d, e, n by the symbol m for a mirror plane.

It is clear that the classification into arithmetic crystal classes refines both the classifications into geometric crystal classes and into Bravais classes, since in the first case only the point groups and in the second case only the translation lattices are taken into account, whereas for the arithmetic crystal classes the combination of point groups and translation lattices is considered. Note, however, that for the determination of the arithmetic crystal class of a space group $\mathcal{G}$ it is not sufficient to look only at the type of the point group and the Bravais type of the translation lattice. It is crucial to consider the action of the point group on the translation lattice.

Example

Let $\mathcal{G}$ and $\mathcal{G}'$ be space groups of types $P3m1$ (156) and $P31m$ (157), respectively. Since $\mathcal{G}$ and $\mathcal{G}'$ are symmorphic space groups of different types, they must belong to different arithmetic classes. The point groups $\mathcal{P}$ and $\mathcal{P}'$ of $\mathcal{G}$ and $\mathcal{G}'$ both belong to the same geometric crystal class with symbol $3m$ and the translation lattices of both space groups are primitive hexagonal lattices, and thus of the same Bravais type. It is the different action on the translation lattice which causes $\mathcal{G}$ and $\mathcal{G}'$ to lie in different arithmetic classes:

In the conventional setting, the point group $\mathcal{P}$ of $\mathcal{G}$ contains the threefold rotation

$$\boldsymbol{R} = \begin{pmatrix} 0 & -1 & 0 \\ 1 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

and the reflections

$$\boldsymbol{M}_1 = \begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \boldsymbol{M}_2 = \begin{pmatrix} -1 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$
$$\text{and } \boldsymbol{M}_3 = \begin{pmatrix} 1 & 0 & 0 \\ 1 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

whereas the point group $\mathcal{P}'$ of $\mathcal{G}'$ contains the same rotation $\boldsymbol{R}$ and the reflections

$$\boldsymbol{M}_1' = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \boldsymbol{M}_2' = \begin{pmatrix} 1 & -1 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$
$$\text{and } \boldsymbol{M}_3' = \begin{pmatrix} -1 & 0 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Since the threefold rotation is represented by the same matrix in both groups, the lattice basis for both groups can be taken as the conventional basis **a**, **b**, **c** of a hexagonal lattice, with **a** and **b** of the same length and enclosing an angle of 120° and **c** perpendicular to the plane spanned by **a** and **b**. One now sees that in $\mathcal{P}'$ the reflection planes of $\boldsymbol{M}_1'$, $\boldsymbol{M}_2'$ and $\boldsymbol{M}_3'$ contain the vectors $\mathbf{a}+\mathbf{b}$, **a** and **b**, respectively, whereas in $\mathcal{P}$ these vectors are just perpendicular to the reflection planes. In the so-called hexagonally centred lattice with primitive basis $\mathbf{a}' = \frac{1}{3}\mathbf{a} + \frac{2}{3}\mathbf{b}$, $\mathbf{b}' = -\frac{2}{3}\mathbf{a} - \frac{1}{3}\mathbf{b}$, $\mathbf{c}' = \mathbf{c}$, the vectors $\mathbf{a}'$ and $\mathbf{b}'$ are perpendicular to the vectors **a** and **b**. The group $\mathcal{G}'$ can thus be regarded as the action of $\mathcal{G}$ on the hexagonally centred lattice, showing that $\mathcal{G}$ and $\mathcal{G}'$ are actions of the same group on different lattices which therefore belong to different arithmetic crystal classes.

As we have seen, the assignment of a space group to its arithmetic crystal class is equivalent to the assignment to its corresponding symmorphic space group, which in turn can be seen as an assignment to the combination of a point group and a lattice on which this point group acts. This correspondence between arithmetic crystal classes and point group/lattice combinations is reflected in the symbol for an arithmetic crystal class suggested in de Wolff *et al.* (1985), which is the symbol of the symmorphic space group with the letter for the lattice moved to the end, *e.g.* $4mmP$ for the arithmetic crystal class containing the symmorphic space groups of type $P4mm$ (99) and the non-symmorphic groups derived from this symmorphic group, *i.e.* the groups of space-group type $P4bm$, $P4_2cm$, $P4_2nm$, $P4cc$, $P4nc$, $P4_2mc$ and $P4_2bc$ (100–106).

Recall that the members of one arithmetic crystal class are space groups with the same translation lattice and the same point group, possibly written with respect to different primitive bases. If the point group happens to be the Bravais group of the translation lattice, this is independent of the chosen primitive basis and thus being a Bravais group is clearly a property of the full arithmetic crystal class.

Definition

The arithmetic crystal class of a space group $\mathcal{G}$ is called a *Bravais arithmetic crystal class* if the point group of $\mathcal{G}$ is the Bravais group of the translation lattice of $\mathcal{G}$.

The arithmetic crystal class of an integral matrix group $\mathcal{P}$ is a Bravais arithmetic crystal class if $\mathcal{P}$ is maximal among the integral matrix groups with the same space of metric tensors $\mathbf{M}(\mathcal{P})$, *i.e.* if for any integral matrix group $\mathcal{P}'$ properly containing $\mathcal{P}$ as a subgroup, the space of metric tensors $\mathbf{M}(\mathcal{P}')$ is strictly smaller than that of $\mathcal{P}$. This amounts to saying that $\mathcal{P}'$ must act on a lattice with specialized metric.

Note that in the previous edition of *IT* A the shorter term *Bravais class* was used as a synonym for Bravais arithmetic crystal class. However, in this edition the term *Bravais class* is reserved for the classification of space-group types according to their lattices (see Section 1.3.4.3).

Since the lattice types are characterized by their Bravais groups, the Bravais arithmetic crystal classes are in one-to-one correspondence with the Bravais types of lattices. The 14 Bravais arithmetic crystal classes (given by the symbol for the arithmetic class, with the number of the associated symmorphic space-group type in brackets) and the corresponding lattice types are: $\bar{1}P$ (2), triclinic; $2/mP$ (10), primitive monoclinic; $2/mC$ (12), centred monoclinic; $mmmP$ (47), primitive orthorhombic; $mmmC$ (65), single-face-centred orthorhombic; $mmmF$ (69), all-face-centred orthorhombic; $mmmI$ (71), body-centred orthorhombic; $4/mmmP$ (123), primitive tetragonal; $4/mmmI$ (139), body-centred tetragonal; $\bar{3}mR$ (166), rhombohedral; $6/mmmP$ (191), hexagonal; $m\bar{3}mP$ (221), primitive cubic; $m\bar{3}mF$ (225), face-centred cubic; and $m\bar{3}mI$ (229), body-centred cubic.

Bravais flocks

In the classification of space groups according to their translation lattices, the point groups play only a secondary role (as groups acting on the lattices). From the perspective of arithmetic crystal classes, this classification can now be reformulated in terms of integral matrix groups. The crucial point is that every arithmetic crystal class can be assigned to a Bravais arithmetic crystal class in a natural way: If $\mathcal{P}$ is a point group, there is a

Table 1.3.4.1
Lattice systems in three-dimensional space

Lattice system	Bravais types of lattices	Holohedry
Triclinic (anorthic)	*aP*	$\bar{1}$
Monoclinic	*mP*, *mS*	2/*m*
Orthorhombic	*oP*, *oS*, *oF*, *oI*	*mmm*
Tetragonal	*tP*, *tI*	4/*mmm*
Hexagonal	*hP*	6/*mmm*
Rhombohedral	*hR*	$\bar{3}m$
Cubic	*cP*, *cF*, *cI*	$m\bar{3}m$

Table 1.3.4.2
Crystal systems in three-dimensional space

Crystal system	Point-group types
Triclinic	$\bar{1}$, 1
Monoclinic	2/*m*, *m*, 2
Orthorhombic	*mmm*, *mm*2, 222
Tetragonal	4/*mmm*, $\bar{4}2m$, 4*mm*, 422, 4/*m*, $\bar{4}$, 4
Hexagonal	6/*mmm*, $\bar{6}2m$, 6*mm*, 622, 6/*m*, $\bar{6}$, 6
Trigonal	$\bar{3}m$, 3*m*, 32, $\bar{3}$, 3
Cubic	$m\bar{3}m$, $\bar{4}3m$, 432, $m\bar{3}$, 23

unique Bravais arithmetic crystal class containing a Bravais group $\mathcal{B}$ of minimal order with $\mathcal{P} \leq \mathcal{B}$. Conversely, a Bravais group $\mathcal{B}$ acting on a lattice $\mathbf{L}$ is grouped together with its subgroups $\mathcal{P}$ that do not act on a more general lattice, *i.e.* on a lattice $\mathbf{L}'$ with more free parameters than $\mathbf{L}$. This observation gives rise to the concept of *Bravais flocks*, which is mainly applied to matrix groups.

Definition

Two integral matrix groups $\mathcal{P}$ and $\mathcal{P}'$ belong to the same Bravais flock if they are both conjugate by an integral basis transformation to subgroups of a common Bravais group, *i.e.* if there exists a Bravais group $\mathcal{B}$ and integral 3×3 matrices $\boldsymbol{P}$ and $\boldsymbol{P}'$ such that $\boldsymbol{PWP}^{-1} \in \mathcal{B}$ for all $\boldsymbol{W} \in \mathcal{P}$ and $\boldsymbol{P}'\boldsymbol{W}'\boldsymbol{P}'^{-1} \in \mathcal{B}$ for all $\boldsymbol{W}' \in \mathcal{P}'$. Moreover, $\mathcal{P}$, $\mathcal{P}'$ and $\mathcal{B}$ must all have spaces of metric tensors of the same dimension.

Each Bravais flock consists of the union of the arithmetic crystal class of a Bravais group $\mathcal{B}$ and the arithmetic crystal classes of the subgroups of $\mathcal{B}$ that do not act on a more general lattice than $\mathcal{B}$.

The classification of space groups into Bravais flocks is the same as that according to the Bravais types of lattices and as that into Bravais classes. If the point groups $\mathcal{P}$ and $\mathcal{P}'$ of two space groups $\mathcal{G}$ and $\mathcal{G}'$ belong to the same Bravais flock, then the space groups are also said to belong to the same Bravais flock, but this is the case if and only if $\mathcal{G}$ and $\mathcal{G}'$ belong to the same Bravais class.

Example

For the body-centred tetragonal lattice the Bravais arithmetic crystal class is the arithmetic crystal class 4/*mmmI* and the corresponding symmorphic space-group type is *I*4/*mmm* (139). The other arithmetic crystal classes in this Bravais flock are (with the number of the corresponding symmorphic space group in brackets): 4*I* (79), $\bar{4}I$ (82), 4/*mI* (87), 422*I* (97), 4*mmI* (107), $\bar{4}m2I$ (119) and $\bar{4}2mI$ (121).

1.3.4.4.2. Lattice systems

It is sometimes convenient to group together those Bravais types of lattices for which the Bravais groups belong to the same holohedry.

Definition

Two lattices belong to the same *lattice system* if their Bravais groups belong to the same geometric crystal class (which is thus a holohedry).

Remark: The lattice systems were called *Bravais systems* in earlier editions of this volume.

Example

The primitive cubic, face-centred cubic and body-centred cubic lattices all belong to the same lattice system, because their Bravais groups all belong to the holohedry with symbol $m\bar{3}m$.

On the other hand, the hexagonal and the rhombohedral lattices belong to different lattice systems, because their Bravais groups are not even of the same order and lie in different holohedries (with symbols 6/*mmm* and $\bar{3}m$, respectively).

From the definition it is obvious that lattice systems classify lattices because they consist of full Bravais types of lattices. On the other hand, the example of the geometric crystal class $\bar{3}m$ shows that lattice systems do not classify point groups, because depending on the chosen basis a point group in this geometric crystal class belongs to either the hexagonal or the rhombohedral lattice system.

However, since the translation lattices of space groups in the same Bravais class belong to the same Bravais type of lattices, the lattice systems can also be regarded as a classification of space groups in which full Bravais classes are grouped together.

Definition

Two Bravais classes belong to the same *lattice system* if the corresponding Bravais arithmetic crystal classes belong to the same holohedry.

More precisely, two space groups $\mathcal{G}$ and $\mathcal{G}'$ belong to the same lattice system if the point groups $\mathcal{P}$ and $\mathcal{P}'$ are contained in Bravais groups $\mathcal{B}$ and $\mathcal{B}'$, respectively, such that $\mathcal{B}$ and $\mathcal{B}'$ belong to the same holohedry and such that $\mathcal{P}$, $\mathcal{P}'$, $\mathcal{B}$ and $\mathcal{B}'$ all have spaces of metric tensors of the same dimension.

Every lattice system contains the lattices of precisely one holohedry and a holohedry determines a unique lattice system, containing the lattices of the Bravais arithmetic crystal classes in the holohedry. Therefore, there is a one-to-one correspondence between holohedries and lattice systems. There are four lattice systems in dimension 2 and seven lattice systems in dimension 3. The lattice systems in three-dimensional space are displayed in Table 1.3.4.1. Along with the name of each lattice system, the Bravais types of lattices contained in it and the corresponding holohedry are given.

1.3.4.4.3. Crystal systems

The point groups contained in a geometric crystal class can act on different Bravais types of lattices, which is the reason why lattice systems do not classify point groups. But the action on different types of lattices can be exploited for a classification of point groups by joining those geometric crystal classes that act on the same Bravais types of lattices. For example, the holohedry $m\bar{3}m$ acts on primitive, face-centred and body-centred cubic lattices. The other geometric crystal classes that act on these three types of lattices are 23, $m\bar{3}$, 432 and $\bar{4}3m$.

Table 1.3.4.3
Distribution of space-group types in the hexagonal crystal family

Crystal system	Geometric crystal class	Lattice system	
		Hexagonal	Rhombohedral
Hexagonal	$6/mmm$	$P6/mmm$, $P6/mcc$, $P6_3/mcm$, $P6_3/mmc$	
	$\bar{6}2m$	$P\bar{6}m2$, $P\bar{6}c2$, $P\bar{6}2m$, $P\bar{6}2c$	
	$6mm$	$P6mm$, $P6cc$, $P6_3cm$, $P6_3mc$	
	622	$P622$, $P6_122$, $P6_522$, $P6_222$, $P6_422$, $P6_322$	
	$6/m$	$P6/m$, $P6_3/m$	
	$\bar{6}$	$P\bar{6}$	
	6	$P6$, $P6_1$, $P6_5$, $P6_2$, $P6_4$, $P6_3$	
Trigonal	$\bar{3}m$	$P\bar{3}1m$, $P\bar{3}1c$, $P\bar{3}m1$, $P\bar{3}c1$	$R\bar{3}m$, $R\bar{3}c$
	$3m$	$P3m1$, $P31m$, $P3c1$, $P31c$	$R3m$, $R3c$
	32	$P312$, $P321$, $P3_112$, $P3_121$, $P3_212$, $P3_221$	$R32$
	$\bar{3}$	$P\bar{3}$	$R\bar{3}$
	3	$P3$, $P3_1$, $P3_2$	$R3$

Definition

Two space groups $\mathcal{G}$ and $\mathcal{G}'$ with point groups $\mathcal{P}$ and $\mathcal{P}'$, respectively, belong to the same *crystal system* if the sets of Bravais types of lattices on which $\mathcal{P}$ and $\mathcal{P}'$ act coincide. Since point groups in the same geometric crystal class act on the same types of lattices, crystal systems consist of full geometric crystal classes and the point groups $\mathcal{P}$ and $\mathcal{P}'$ are also said to belong to the same crystal system.

Remark: In the literature there are many different notions of crystal systems. In *International Tables*, only the one defined above is used.

In many cases, crystal systems collect together geometric crystal classes for point groups that are in a group–subgroup relation and act on lattices with the same number of free parameters. However, this condition is not sufficient. If a point group $\mathcal{P}$ is a subgroup of another point group $\mathcal{P}'$, it is clear that $\mathcal{P}$ acts on each lattice on which $\mathcal{P}'$ acts. But $\mathcal{P}$ may in addition act on different types of lattices on which $\mathcal{P}'$ does not act.

Note that it is sufficient to consider the action on lattices with the maximal number of free parameters, since the action on these lattices implies the action on lattices with a smaller number of free parameters (corresponding to metric specializations).

Example

The holohedry of type $4/mmm$ acts on tetragonal and body-centred tetragonal lattices. The crystal system containing this holohedry thus consists of all the geometric crystal classes in which the point groups act on tetragonal and body-centred tetragonal lattices, but not on lattices with more than two free parameters. This is the case for all geometric crystal classes with point groups containing a fourfold rotation or rotoinversion and that are subgroups of a point group of type $4/mmm$. This means that the crystal system containing the holohedry $4/mmm$ consists of the geometric classes of types 4, $\bar{4}$, $4/m$, 422, $4mm$, $\bar{4}2m$ and $4/mmm$.

This example is typical for the situation in three-dimensional space, since in three-dimensional space usually all the arithmetic crystal classes contained in a holohedry are Bravais arithmetic crystal classes. In this case, the geometric crystal classes in the crystal system of the holohedry are simply the classes of those subgroups of a point group in the holohedry that do not act on lattices with a larger number of free parameters.

The only exceptions from this situation are the Bravais arithmetic crystal classes for the hexagonal and rhombohedral lattices.

Example

A point group containing a threefold rotation but no sixfold rotation or rotoinversion acts both on a hexagonal lattice and on a rhombohedral lattice. On the other hand, point groups containing a sixfold rotation only act on a hexagonal but not on a rhombohedral lattice. The geometric crystal classes of point groups containing a threefold rotation or rotoinversion but not a sixfold rotation or rotoinversion form a crystal system which is called the *trigonal crystal system*. The geometric crystal classes of point groups containing a sixfold rotation or rotoinversion form a different crystal system, which is called the *hexagonal crystal system*.

The classification of the point-group types into crystal systems is summarized in Table 1.3.4.2.

Remark: Crystal systems can contain at most one holohedry and in dimensions 2 and 3 it is true that every crystal system does contain a holohedry. However, this is not true in higher dimensions. The smallest counter-examples exist in dimension 5, where two (out of 59) crystal systems do not contain any holohedry.

1.3.4.4.4. Crystal families

The classification into crystal systems has many important applications, but it has the disadvantage that it is not compatible with the classification into lattice systems. Space groups that belong to the hexagonal lattice system are distributed over the trigonal and the hexagonal crystal system. Conversely, space groups in the trigonal crystal system belong to either the rhombohedral or the hexagonal lattice system. It is therefore desirable to define a further classification level in which the classes consist of full crystal systems and of full lattice systems, or, equivalently, of full geometric crystal classes and full Bravais classes. Since crystal systems already contain only geometric crystal classes with spaces of metric tensors of the same dimension, this can be achieved by the following definition.

Definition

For a space group $\mathcal{G}$ with point group $\mathcal{P}$ the *crystal family* of $\mathcal{G}$ is the union of all geometric crystal classes that contain a space group $\mathcal{G}'$ that has the same Bravais type of lattices as $\mathcal{G}$.

The crystal family of $\mathcal{G}$ thus consists of those geometric crystal classes that contain a point group $\mathcal{P}'$ such that $\mathcal{P}$ and $\mathcal{P}'$ are contained in a common supergroup $\mathcal{B}$ (which is a Bravais group) and such that $\mathcal{P}$, $\mathcal{P}'$ and $\mathcal{B}$ all act on lattices with the same number of free parameters.

In two-dimensional space, the crystal families coincide with the crystal systems and in three-dimensional space only the trigonal and hexagonal crystal system are merged into a single crystal family, whereas all other crystal systems again form a crystal family on their own.

Example

The trigonal and hexagonal crystal systems belong to a single crystal family, called the *hexagonal crystal family*, because for both crystal systems the number of free parameters of the corresponding lattices is 2 and a point group of type $\bar{3}m$ in the trigonal crystal system is a subgroup of a point group of type $6/mmm$ in the hexagonal crystal system.

A space group in the hexagonal crystal family belongs to either the trigonal or the hexagonal crystal system and to either the rhombohedral or the hexagonal lattice system. A group in the hexagonal crystal system cannot belong to the rhombohedral lattice system, but all other combinations of crystal system and lattice system are possible. The distribution of the space groups in the hexagonal crystal family over these different combinations is displayed in Table 1.3.4.3.

Remark: Up to dimension 3 it seems exceptional that a crystal family contains more than one crystal system, since the only instance of this phenomenon is the hexagonal crystal family consisting of the trigonal and the hexagonal crystal systems. However, in higher dimensions it actually becomes rare that a crystal family consists only of a single crystal system.

For the space groups within one crystal family the same coordinate system is usually used, which is called the *conventional coordinate system* (for this crystal family). However, depending on the application it may be useful to work with a different coordinate system. To avoid confusion, it is recommended to state explicitly when a coordinate system differing from the conventional coordinate system is used.

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