International Tables for Crystallography (2016). Vol. A, Section 1.3.4.3, pp. 34–37.

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

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.* $\boldsymbol{W}^{\mathrm{T}} \cdot \boldsymbol{G} \cdot \boldsymbol{W} = \boldsymbol{G}$ 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 $\alpha = \beta = \gamma = 90^\circ$ 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

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

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 $\mathcal{B} = Aut(\mathbf{L}) = \{\boldsymbol{W} \in {\rm GL}_3(\mathbb{Z}) \mid \boldsymbol{W}^{\rm T} \cdot \boldsymbol{G} \cdot \boldsymbol{W} = \boldsymbol{G}\}$ be the Bravais group of $\mathbf{L}$. Then

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

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 $\mathcal{P}$,

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

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 corre-