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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 **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 **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 $\mathbf{a}, \mathbf{b}, \mathbf{c}$ of a hexagonal lattice, with $\mathbf{a}$ and $\mathbf{b}$ of the same length and enclosing an angle of 120° and $\mathbf{c}$ perpendicular to the plane spanned by $\mathbf{a}$ and $\mathbf{b}$. One now sees that in $\mathcal{P}'$ the reflection planes of $\boldsymbol{M}'_1$, $\boldsymbol{M}'_2$ and $\boldsymbol{M}'_3$ contain the vectors $\mathbf{a}+\mathbf{b}$, $\mathbf{a}$ and $\mathbf{b}$, 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 $\mathbf{a}$ and $\mathbf{b}$. 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	$m\bar{3}m$

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 $I4/mmm$ (139). The other arithmetic crystal classes in this Bravais flock are (with the number of the corresponding symmorphic space group in brackets): $4I$ (79), $\bar{4}I$ (82), $4/mI$ (87), $422I$ (97), $4mmI$ (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).

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, $mm2$, 222
Tetragonal	$4/mmm$, $\bar{4}2m$, $4mm$, 422, $4/m$, $\bar{4}$, 4
Hexagonal	$6/mmm$, $\bar{6}2m$, $6mm$, 622, $6/m$, $\bar{6}$, 6
Trigonal	$\bar{3}m$, $3m$, 32, $\bar{3}$, 3
Cubic	$m\bar{3}m$, $\bar{4}3m$, 432, $m\bar{3}$, 23

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 $\bar{4}3m$.