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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	$4/mmm$, $\bar{4}2m$, $4mm$, 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

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 $\boldsymbol{P}\boldsymbol{W}\boldsymbol{P}^{-1} \in \mathcal{B}$ 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).

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.