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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.

References

Armstrong, M. A. (1997). *Groups and Symmetry*. New York: Springer.

Bieberbach, L. (1911). *Über die Bewegungsgruppen der Euklidischen Räume. (Erste Abhandlung)*. *Math. Ann.* **70**, 297–336.

Bieberbach, L. (1912). *Über die Bewegungsgruppen der Euklidischen Räume. (Zweite Abhandlung). Die Gruppen mit einem endlichen Fundamentalbereich*. *Math. Ann.* **72**, 400–412.

Minkowski, H. (1887). *Zur Theorie der positiven quadratischen Formen. J. Reine Angew. Math.* **101**, 196–202.

Wolff, P. M. de, Belov, N. V., Bertaut, E. F., Buerger, M. J., Donnay, J. D. H., Fischer, W., Hahn, Th., Koptsik, V. A., Mackay, A. L., Wondratschek, H., Wilson, A. J. C. & Abrahams, S. C. (1985). *Nomenclature for crystal families, Bravais-lattice types and arithmetic classes. Report of the International Union of Crystallography Ad-Hoc Committee on the Nomenclature of Symmetry*. *Acta Cryst.* A**41**, 278–280.