

## 1.3. GENERAL INTRODUCTION TO SPACE GROUPS

**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  $3 \times 3$  matrices  $\mathbf{P}$  and  $\mathbf{P}'$  such that  $\mathbf{P}\mathbf{W}\mathbf{P}^{-1} \in \mathcal{B}$  for all  $\mathbf{W} \in \mathcal{P}$  and  $\mathbf{P}'\mathbf{W}'\mathbf{P}'^{-1} \in \mathcal{B}$  for all  $\mathbf{W}' \in \mathcal{P}'$ . 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),  $4m2I$  (119) and  $42mI$  (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

**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	$m\bar{3}m, \bar{4}3m, 432, m\bar{3}, 23$

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  $\bar{4}3m$ .