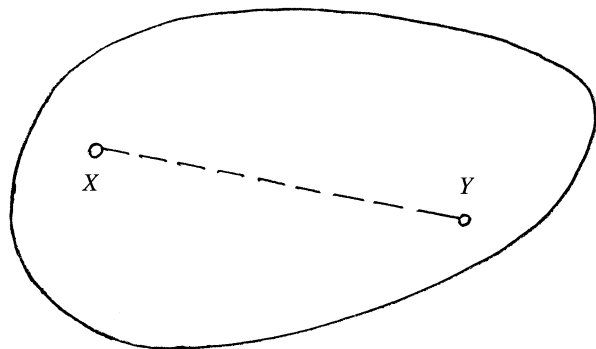


9.3. FURTHER PROPERTIES OF LATTICES

Fig. 9.3.2.2. A convex set in E_2 .

We say that two lattices of the same Bravais type belong to the same lattice character if one of them can be deformed into the other in such a way that the Niggli point of the deformed lattice moves *linearly* from the initial to the final position while the Bravais type of the lattice remains unchanged.

Unlike convexity, nothing can be said whether the Niggli images of lattice characters are *open sets* (with regard to their dimension) or not. Both cases occur.

The lattice character of a lattice L can also be recognized [instead of by means of Table 9.2.5.1 or by Tables 1 and 3 in Gruber (1992)] by perpendicular projection of the \mathbf{c} vector onto the \mathbf{ab} plane provided the vectors \mathbf{a} , \mathbf{b} , \mathbf{c} describe the Niggli cell of L and fulfil the conditions (9.2.2.2a) to (9.2.2.5f) in Section 9.2.2 (de Wolff & Gruber, 1991). See also Figs. 9.2.4.1 to 9.2.4.5.

9.3.3. A finer division of lattices

The 44 lattice characters form a subdivision of the 14 Bravais types. There is another commonly known subdivision of the Bravais types, namely the 24 Delaunay sorts (*symmetrische Sorten*) (Delaunay, 1933; *International Tables for X-ray Crystallography*, 1952, Vol. I; cf. Section 9.1.8). However, both divisions, being based on quite different principles, are incompatible: the 44 lattice characters do not form a subdivision of the 24 Delaunay sorts.

A natural problem arises to construct a division of lattices which would be a subdivision of both the lattice characters and the Delaunay sorts. However, we do not admit a purely mechanical intersection of both these divisions; we insist that their common subdivision be crystallographically meaningful.

Such a division was proposed recently (Gruber, 1997a). It uses the fact that the Niggli points of all lattices lie in two five-dimensional polyhedra, say Ω^+ and Ω^- . The underlying idea, originating from H. Wondratschek, is based on the distribution of Niggli points among the vertices, edges, faces, three- and four-dimensional hyperfaces, and the interior of Ω^+ and Ω^- . This leads to a natural division of Niggli points and further to a division of lattices. This division has 67 classes, but is not suitable for crystallography because it does not constitute a subdivision of the Bravais types.

A modification of the idea is necessary. It consists of representing a lattice L by several points (instead of by one Niggli point) and the addition of two minor conditions. One of them concerns the diagonals of the Niggli cell and the other the bases of L which describe the Niggli cell.

Though these conditions are of little importance in themselves, they lead to a very useful notion, *viz* the division of all lattices into 127 classes which is a subdivision of both the lattice characters and

the Delaunay sorts. The equivalence classes of this division are called *genera*. They form, in a certain sense, building blocks of both lattice characters and Delaunay sorts and show their mutual relationship.

The distribution of genera along the Bravais types is the following (the number of genera is given in parentheses): $cP(1)$, $cI(1)$, $cF(1)$, $tP(2)$, $tI(5)$, $oP(1)$, $oC(8)$, $oI(7)$, $oF(3)$, $hP(3)$, $hR(4)$, $mP(5)$, $mC(43)$, $aP(43)$. Thus, genera seem to be especially suitable for a finer classification of lattices of low symmetry.

The genus of a given lattice L can be determined – provided that the Niggli point of L is known – by means of a table containing explicit descriptions of all genera. These descriptions are formed by open linear systems of inequalities. Consequently, the ranges of conventional parameters of genera are open unlike those concerning the lattice characters.

Genera are denoted by symbols derived from the geometrical shape of Ω^+ and Ω^- . They can be visualized in the three-dimensional cross sections of these bodies. This gives a fairly good illustration of the relationships between genera.

However, the most important feature of genera seems to be the fact that lattices of the same genus agree in a surprisingly great number of crystallographically significant properties, such as the number of Buerger cells, the densest directions and planes, the symmetry of these planes *etc.* Even the formulae for the conventional cells are the same. The genus appears to be a remarkably strong bond between lattices.

9.3.4. Conventional cells

Conventional cells are dealt with in Chapter 9.1. They are illustrated in Fig. 9.1.7.1 and described in Table 9.1.7.2. This description, however, is not exhaustive enough for determining the Bravais type. In mathematical terms, the conditions in Table 9.1.7.2 are necessary but not sufficient. For example, the C -centred cell with

$$a = 6, \quad b = 8, \quad c = 5, \quad \cos \beta = -7/15, \quad \alpha = \gamma = 90^\circ \quad (9.3.4.1)$$

has the typical shape of a conventional cell of an mC lattice. But the lattice generated by the C -centred cell (9.3.4.1) is actually hR with the conventional rhombohedral basis vectors

$$\mathbf{c}, \quad (\mathbf{a} + \mathbf{b})/2, \quad (\mathbf{a} - \mathbf{b})/2.$$

It is a natural goal to establish a system of conditions for the conventional cells which would be not only necessary but also sufficient. This is done in Table 9.3.4.1. In order to make the conditions as simple as possible, the usual mC description of the monoclinic centred lattices is replaced by the mI description. The relation between the two descriptions is simple:

$$\mathbf{a}_I = -\mathbf{c}_C, \quad \mathbf{b}_I = \mathbf{b}_C, \quad \mathbf{c}_I = \mathbf{a}_C + \mathbf{c}_C.$$

The exact meaning of Table 9.3.4.1 is as follows: Suppose that a Bravais type different from aP is given and that its symbol appears in column 1 in the i th entry of Table 9.3.4.1. Then a lattice L is of this Bravais type if and only if there exists a cell $(\mathbf{a}, \mathbf{b}, \mathbf{c})$ in L such that

- (i) the centring of $(\mathbf{a}, \mathbf{b}, \mathbf{c})$ agrees with the centring mode given in column 2 in the i th entry, and
- (ii) the parameters of the cell $(\mathbf{a}, \mathbf{b}, \mathbf{c})$ fulfil the conditions listed in column 3 in the i th entry of Table 9.3.4.1.

9.3.5. Conventional characters

Lattice characters were defined in Section 9.3.2 by dividing the Niggli image of a certain Bravais type \mathcal{F} into components. Doing

9. CRYSTAL LATTICES

Table 9.3.4.1. Conventional cells

Bravais type	Centring mode of the cell (a , b , c)	Conditions
<i>cP</i>	<i>P</i>	$a = b = c,$ $\alpha = \beta = \gamma = 90^\circ$
<i>cI</i>	<i>I</i>	$a = b = c,$ $\alpha = \beta = \gamma = 90^\circ$
<i>cF</i>	<i>F</i>	$a = b = c,$ $\alpha = \beta = \gamma = 90^\circ$
<i>tP</i>	<i>P</i>	$a = b \neq c,$ $\alpha = \beta = \gamma = 90^\circ$
<i>tI</i>	<i>I</i>	$c/\sqrt{2} \neq a = b \neq c,^*$ $\alpha = \beta = \gamma = 90^\circ$
<i>oP</i>	<i>P</i>	$a < b < c,^\dagger$ $\alpha = \beta = \gamma = 90^\circ$
<i>oI</i>	<i>I</i>	$a < b < c,$ $\alpha = \beta = \gamma = 90^\circ$
<i>oF</i>	<i>F</i>	$a < b < c,$ $\alpha = \beta = \gamma = 90^\circ$
<i>oC</i>	<i>C</i>	$a < b \neq a\sqrt{3},^\ddagger$ $\alpha = \beta = \gamma = 90^\circ$
<i>hP</i>	<i>P</i>	$a = b,$ $\alpha = \beta = 90^\circ, \gamma = 120^\circ$
<i>hR</i>	<i>P</i>	$a = b = c,$ $\alpha = \beta = \gamma,$ $\alpha \neq 60^\circ, \alpha \neq 90^\circ, \alpha \neq \omega^\S$
<i>mP</i>	<i>P</i>	$-2c \cos \beta < a < c,^\P$ $\alpha = \gamma = 90^\circ < \beta$
<i>mI</i>	<i>I</i>	$-c \cos \beta < a < c,^{**}$ $\alpha = \gamma = 90^\circ < \beta,$ (9.3.4.2) but not $a^2 + b^2 = c^2,$ $a^2 + ac \cos \beta = b^2,^\ddagger\ddagger$ (9.3.4.3) nor $a^2 + b^2 = c^2,$ $b^2 + ac \cos \beta = a^2,^\ddagger\ddagger$ (9.3.4.4) nor $c^2 + 3b^2 = 9a^2,$ $c = -3a \cos \beta,^\S\S$ (9.3.4.5) nor $a^2 + 3b^2 = 9c^2,$ $a = -3c \cos \beta,^\P\P$ (9.3.4.6)

Note: All remaining cases are covered by Bravais type *aP*.

* For $a = c/\sqrt{2}$, the lattice is *cF* with conventional basis vectors **c**, **a + b**, **a - b**.
 † The labelling of the basis vectors according to their length is the reason for unconventional Hermann–Mauguin symbols: for example, the Hermann–Mauguin symbol *Pmna* may be changed to *Pncm*, *Pbmn*, *Pman*, *Pcnm* or *Pnmb*. Analogous facts apply to the *oI*, *oC*, *oF*, *mP* and *mI* Bravais types.
 ‡ For $b = a\sqrt{3}$, the lattice is *hP* with conventional vectors **a**, **(b - a)/2**, **c**.
 § $\omega = \arccos(-1/3) = 109^\circ 28' 16''$. For $\alpha = 60^\circ$, the lattice is *cF* with conventional vectors $-\mathbf{a} + \mathbf{b} + \mathbf{c}$, $\mathbf{a} - \mathbf{b} + \mathbf{c}$, $\mathbf{a} + \mathbf{b} - \mathbf{c}$; for $\alpha = \omega$, the lattice is *cI* with conventional vectors **a + b**, **a + c**, **b + c**.
 ¶ This means that **a**, **c** are shortest non-coplanar lattice vectors in their plane.
 ** This means that **a**, **c** are shortest non-coplanar lattice vectors in their plane on condition that the cell (**a**, **b**, **c**) is body-centred.
 †† If (9.3.4.2) and (9.3.4.3) hold, the lattice is *hR* with conventional vectors **a**, **(a + b - c)/2**, **(a - b - c)/2**, making the rhombohedral angle smaller than 60° .
 ‡‡ If (9.3.4.2) and (9.3.4.4) hold, the lattice is *hR* with conventional vectors **a**, **(a + b + c)/2**, **(a - b + c)/2**, making the rhombohedral angle between 60 and 90° .
 §§ If (9.3.4.2) and (9.3.4.5) hold, the lattice is *hR* with conventional vectors $-\mathbf{a}$, **(a + b + c)/2**, **(a - b + c)/2**, making the rhombohedral angle between 90° and ω .
 ¶¶ If (9.3.4.2) and (9.3.4.6) hold, the lattice is *hR* with conventional vectors $-\mathbf{c}$, **(a + b + c)/2**, **(a - b + c)/2**, making the rhombohedral angle greater than ω .

Table 9.3.5.1. Conventional characters

Bravais type	Conditions	Conventional character
<i>cP</i>		{3}
<i>cI</i>		{5}
<i>cF</i>		{1}
<i>tP</i>	$a < c$	{11}
	$c < a$	{21}
<i>tI</i>	$a < c/\sqrt{2}$	{15}
	$c/\sqrt{2} < a < c$	{7}
	$c < a$	{6, 18}
<i>oP</i>		{32}
<i>oI</i>		{8, 19, 42}
<i>oF</i>		{16, 26}
<i>oC</i>	$b < a\sqrt{3}$	{13, 23}
	$a\sqrt{3} < b$	{36, 38, 40}
<i>hP</i>		{12, 22}
<i>hR*</i>	$\alpha < 60^\circ$	{9}
	$60^\circ < \alpha < 90^\circ$	{2}
	$90^\circ < \alpha < \omega^\dagger$	{4}
	$\omega < \alpha$	{24}
<i>mP</i>		{33, 34, 35}
<i>mC</i>		{10, 14, 17, 20, 25, 27, 28, 29, 30, 37, 39, 41, 43}
<i>aP</i>	$\alpha < 90^\circ$	{31}
	$90^\circ \leq \alpha$	{44}

* The angle α refers to the rhombohedral description of the *hR* lattices.
 † $\omega = \arccos(-1/3) = 109^\circ 28' 16''$.

the same – instead of with the Niggli points – with the parameters of conventional cells* of lattices of the Bravais type \mathcal{F} we obtain a division of the range† of these parameters into components. This leads to a further division of lattices of the Bravais type \mathcal{F} into equivalence classes. We call these classes – in analogy to the Niggli characters – *conventional characters*. There are 22 of them.

Two lattices of the same Bravais type belong to the same conventional character if and only if one lattice can be deformed into the other in such a way that the conventional parameters of the deformed lattice change *continuously* from the initial to the final position without change of the Bravais type. The word ‘continuously’ cannot be replaced by the stronger term ‘linearly’ because the range of conventional parameters of the monoclinic centred lattices is not convex.

Conventional characters form a superdivision of the lattice characters. Therefore, no special notation of conventional characters need be invented: we write them simply as sets of lattice characters which constitute the conventional character. Denoting the lattice characters by integral numbers from 1 to 44 (according to the convention in Section 9.2.5), we obtain for the conventional characters symbols like {8, 19, 42} or {7}.

Conventional characters are described in Table 9.3.5.1.

9.3.6. Sublattices

A sublattice L' of an n -dimensional lattice L is a proper subset of L which itself is a lattice of the same dimension as L . A sublattice L' of

* For *aP* lattices, these parameters are derived from the Niggli point [see (9.3.2.1)].
 † This range is a subset of E_k , where $k \leq 6$.