Table 9.3.4.1. *Conventional cells*

Bravais type	Centring mode of the cell (**a**, **b**, **c**)	Conditions
cP	*P*	$a = b = c$, $\alpha = \beta = \gamma = 90°$
cI	*I*	$a = b = c$, $\alpha = \beta = \gamma = 90°$
cF	*F*	$a = b = c$, $\alpha = \beta = \gamma = 90°$
tP	*P*	$a = b \neq c$, $\alpha = \beta = \gamma = 90°$
tI	*I*	$c/\sqrt{2} \neq a = b \neq c$,* $\alpha = \beta = \gamma = 90°$
oP	*P*	$a < b < c$,† $\alpha = \beta = \gamma = 90°$
oI	*I*	$a < b < c$, $\alpha = \beta = \gamma = 90°$
oF	*F*	$a < b < c$, $\alpha = \beta = \gamma = 90°$
oC	*C*	$a < b \neq a\sqrt{3}$,‡ $\alpha = \beta = \gamma = 90°$
hP	*P*	$a = b$, $\alpha = \beta = 90°,\ \gamma = 120°$
hR	*P*	$a = b = c$, $\alpha = \beta = \gamma$, $\alpha \neq 60°,\ \alpha \neq 90°,\ \alpha \neq \omega$§
mP	*P*	$-2c\cos\beta < a < c$,¶ $\alpha = \gamma = 90° < \beta$
mI	*I*	$-c\cos\beta < a < c$,** $\alpha = \gamma = 90° < \beta$, (9.3.4.2) but not $a^2 + b^2 = c^2$, $a^2 + ac\cos\beta = b^2$,†† (9.3.4.3) nor $a^2 + b^2 = c^2$, $b^2 + ac\cos\beta = a^2$,‡‡ (9.3.4.4) nor $c^2 + 3b^2 = 9a^2$, $c = -3a\cos\beta$,§§ (9.3.4.5) nor $a^2 + 3b^2 = 9c^2$, $a = -3c\cos\beta$¶¶ (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 $\mathbf{c}, \mathbf{a}+\mathbf{b}, \mathbf{a}-\mathbf{b}$.
† 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 $\mathbf{a}, (\mathbf{b}-\mathbf{a})/2, \mathbf{c}$.
§ $\omega = \arccos(-1/3) = 109°28'16''$. For $\alpha = 60°$, 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 $\mathbf{a}+\mathbf{b}, \mathbf{a}+\mathbf{c}, \mathbf{b}+\mathbf{c}$.
¶ 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 $\mathbf{a}, (\mathbf{a}+\mathbf{b}-\mathbf{c})/2, (\mathbf{a}-\mathbf{b}-\mathbf{c})/2$, 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 $\mathbf{a}, (\mathbf{a}+\mathbf{b}+\mathbf{c})/2, (\mathbf{a}-\mathbf{b}+\mathbf{c})/2$, 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 $-\mathbf{a}, (\mathbf{a}+\mathbf{b}+\mathbf{c})/2, (\mathbf{a}-\mathbf{b}+\mathbf{c})/2$, 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 $-\mathbf{c}, (\mathbf{a}+\mathbf{b}+\mathbf{c})/2, (\mathbf{a}-\mathbf{b}+\mathbf{c})/2$, making the rhombohedral angle greater than ω.

Table 9.3.5.1. *Conventional characters*

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

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

the same – instead of with the Niggli points – with the parameters of conventional cells* of lattices of the Bravais type $\mathscr{T}$ we obtain a division of the range† of these parameters into components. This leads to a further division of lattices of the Bravais type $\mathscr{T}$ 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 $k \leq 6$.

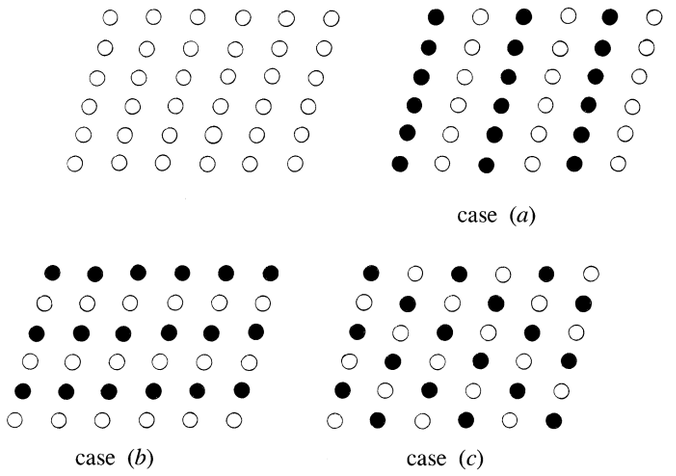

Fig. 9.3.6.1. Three possible decompositions of a two-dimensional lattice L into sublattices of index 2.

L causes a decomposition of the set L into, say, i mutually congruent sublattices, L' itself being one of them (Fig. 9.3.6.1). The number i is called the *index* of the sublattice L' and indicates how many times L' is 'diluted' with respect to L.

Sublattices are defined in a natural way in those lattices that have centred conventional cells, being generated by the vertices of these cells ('decentring'). They are primitive and belong to the same crystal family as the given lattice. Thus, in the *cI*, *cF*, *tI*, *oI*, *oF*, *oC*, *mC* and *hR* * lattices, we can meet sublattices of indices 2, 4, 2, 2, 4, 2, 2 and 3, respectively.

Theoretically (though hardly in crystallographic practice), the Bravais type of centred lattices can also be determined by testing all their sublattices with the suspected index and finding in any of these sublattices the Niggli cell.

All sublattices of index i of an n-dimensional lattice L can be constructed by a procedure suggested by Cassels (1971). If $\mathbf{a}_1, \ldots, \mathbf{a}_n$ is a primitive basis of the lattice L then primitive bases $\mathbf{a}'_1, \ldots, \mathbf{a}'_n$ of all sublattices of index i of the lattice L can be found by the relations

$$[\mathbf{a}'_1, \ldots, \mathbf{a}'_n] = [\mathbf{a}_1, \ldots, \mathbf{a}_n]\boldsymbol{R}^T,$$

where the matrix $\boldsymbol{R} = [r_{ij}]$ fulfils

$$\begin{aligned} 0 &= r_{ij} && \text{for} \quad 1 \le i < j \le n, \\ 0 &\le r_{ij} < r_{jj} && \text{for} \quad 1 \le j < i \le n, \\ r_{11} \ldots r_{nn} &= i. \end{aligned} \tag{9.3.6.1}$$

The number $D_{n,i}$ of these matrices is equal to the number of decompositions of an n-dimensional lattice L into sublattices of index i. To determine this number, it is not necessary to construct explicitly the matrices fulfilling (9.3.6.1). The following formulae (Gruber, 1997*b*) can be used:

(i) If $i = p^q$, where $p > 1$ is a prime number, then

$$D_{n,i} = \underbrace{\frac{p^n - 1}{p - 1} \times \frac{p^{n+1} - 1}{p^2 - 1} \times \frac{p^{n+2} - 1}{p^3 - 1} \times \ldots}_{q \text{ times}}$$

(ii) If $i = p_1^{q_1} \ldots p_m^{q_m}$ ($p_1, \ldots, p_m$ mutually different prime numbers, $m > 1$), we deal with any factor $p_j^{q_j}$ ($j = 1, \ldots, m$) according to point (i) and multiply all these numbers to obtain the number $D_{n,i}$.

For example, for $n = 3$ and i = 2, 3, 4 and 6, we obtain for $D_{n,i}$ the values 7, 13, 35 and 91, respectively.

In all considerations so far, the symmetry of the lattice L was irrelevant. We took L simply as a set of points and its sublattices as its subsets. (Thus, for illustrating sublattices, the 'triclinic' lattices are most apt; *cf.* 'derivative lattices' in Chapter 13.2.)

However, this is not exactly the crystallographic point of view. If, for example, the mesh of the lattice L in Fig. 9.3.6.1 were a square, the sublattices in cases (*a*) and (*b*) would have the same symmetry (though being different subsets of L) and therefore would be considered by crystallographers as one case only. The number $D_{n,i}$ would be reduced. From this aspect, the problem is treated in Chapter 13.1 in group-theoretical terms which are more suitable for this purpose than the set-theory language used here.

* When choosing their hexagonal description.

references