

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 $k \leq 6$.