

3. ADVANCED TOPICS ON SPACE-GROUP SYMMETRY

Table 3.1.4.3
Conventional characters

Bravais type of lattice	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}
	$90^\circ < \alpha < \omega^\ddagger$	{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. [‡] $\omega = \arccos(-1/3) = 109^\circ 28' 16''$.

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 3.1.3.5), we obtain for the conventional characters symbols like {8, 19, 42} or {7}.

Conventional characters are described in Table 3.1.4.3.

3.1.4.6. 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 **L** causes a decomposition of the set **L** into, say, *i* mutually congruent sublattices, **L'** itself being one of them (Fig. 3.1.4.5). 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*⁹ 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 **a**₁, ..., **a**_{*n*} is a primitive basis of the lattice **L** then primitive bases **a'**₁, ..., **a'**_{*n*} of all sublattices of index *i* of the lattice **L** can be found by the relations

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

⁹ When choosing their hexagonal description.

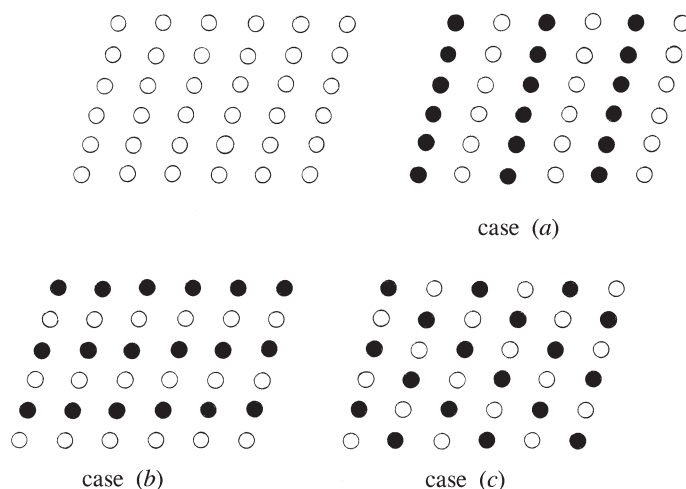


Figure 3.1.4.5
Three possible decompositions of a two-dimensional lattice **L** into sublattices of index 2.

where the matrix **R** = [*r*_{*ij*}] fulfils

$$\begin{aligned} 0 &= r_{ij} && \text{for } 1 \leq i < j \leq n, \\ 0 &\leq r_{ij} < r_{jj} && \text{for } 1 \leq j < i \leq n, \\ r_{11} \dots r_{nn} &= i. \end{aligned} \tag{3.1.4.4}$$

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 (3.1.4.4). The following formulae (Gruber, 1997b) can be used:

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

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

(ii) If *i* = *p*₁^{*q*₁} ... *p*_{*m*}^{*q*_{*m*}} (*p*₁, ..., *p*_{*m*} mutually different prime numbers, *m* > 1), we deal with any factor *p*_{*j*}^{*q*_{*j*}} (*j* = 1, ..., *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 in the 5th (2002) edition of this volume.]

However, this is not exactly the crystallographic point of view. If, for example, the mesh of the lattice **L** in Fig. 3.1.4.5 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 the 5th (2002) edition of this volume in group-theoretical terms which are more suitable for this purpose than the set-theory language used here. See also Section 2.1.4 of *International Tables for Crystallography* Volume A1 (2010).

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