International Tables for Crystallography (2006). Vol. A, Chapter 9.3, pp. 756–760.

9.3. Further properties of lattices

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9.3.1. Further kinds of reduced cells

In Section 9.2.2, a 'reduced basis' of a lattice is defined which permits a unique representation of this lattice. It was introduced into crystallography by Niggli (1928) and incorporated into *International Tables for X-ray Crystallography* (1969), Vol. I. Originating from algebra (Eisenstein, 1851), a reduced basis is defined in a rather complicated manner [conditions (9.2.2.2*a*) to (9.2.2.5*f*) in Section 9.2.2] and lacks any geometrical meaning. A cell spanned by a reduced basis is called the *Niggli cell*.

However, unique primitive cells may be introduced also in other ways that – unlike the Niggli cell* – have significant geometrical features based mainly on extremal principles (Gruber, 1989). We shall describe some of them below.

If a (primitive) cell of the lattice L fulfils the condition

$$a + b + c = \min$$

on the set of all primitive cells of L, we call it a *Buerger cell*. This cell need not be unique with regard to its shape in the lattice. There exist lattices with 1, 2, 3, 4 and 5 (but not more) Buerger cells differing in shape. The uniqueness can be achieved by various additional conditions. In this way, we can arrive at the following four reduced cells:

(i) the Buerger cell with minimum surface;†
(ii) the Buerger cell with maximum surface;
(iii) the Buerger cell with minimum deviation;‡
(iv) the Buerger cell with maximum deviation.

Equivalent definitions can be obtained by replacing the term 'surface' in (i) and (ii) by the expression

$$\sin\alpha + \sin\beta + \sin\gamma$$

or

$$\sin\alpha \sin\beta \sin\gamma,$$

and by replacing the 'deviation' in (iii) and (iv) by

$$|\cos\alpha| + |\cos\beta| + |\cos\gamma|$$

or

$$|\cos\alpha \cos\beta \cos\gamma|.$$

A Buerger cell can agree with more than one of the definitions

$$\text{(i)},\ \text{(ii)},\ \text{(iii)},\ \text{(iv)}. \qquad (9.3.1.1)$$

For example, if a lattice has only one Buerger cell, then this cell agrees with all the definitions in (9.3.1.1). However, there exist also Buerger cells that are in agreement with none of them. Thus, the definitions (9.3.1.1) do not imply a partition of Buerger cells into classes.

It appears that case (iv) coincides with the Niggli cell. This is important because this cell can now be defined by a simple geometrical property instead of a complicated system of conditions.

Further reduced cells can be obtained by applying the definitions (9.3.1.1) to the reciprocal lattice. Then, to a Buerger cell in the reciprocal lattice, there corresponds a primitive cell with absolute minimum surface§ in the direct lattice.

The reduced cells according to the definitions (9.3.1.1) can be recognized by means of a table and found in the lattice by means of algorithms. Detailed mutual relationships between them have been ascertained.

9.3.2. Topological characteristic of lattice characters

In his thorough analysis of lattice characters, de Wolff (1988) remarks that so far they have not been defined as clearly as the Bravais types and that an exact general definition does not exist. Gruber (1992) tried to base such a definition on topological concepts.

The crucial notion is the decomposition of a set $\boldsymbol{M}$ of points of the n-dimensional Euclidean space E_n into equivalence classes called *components* of the set $\boldsymbol{M}$. They can be defined as follows: Two points X,Y of the set $\boldsymbol{M}$ belong to the same component if they can be connected by a *continuous* path which lies entirely in the set $\boldsymbol{M}$ (Fig. 9.3.2.1). This partition of the set $\boldsymbol{M}$ into components is unique and is determined solely by the set $\boldsymbol{M}$.

Now let us return to lattices. To any lattice L there is attached a point in E_5 called the *Niggli point* of L. It is the point

$$\left[\frac{\mathbf{a}\cdot\mathbf{a}}{\mathbf{c}\cdot\mathbf{c}}, \frac{\mathbf{b}\cdot\mathbf{b}}{\mathbf{c}\cdot\mathbf{c}}, \frac{2\mathbf{b}\cdot\mathbf{c}}{\mathbf{c}\cdot\mathbf{c}}, \frac{2\mathbf{a}\cdot\mathbf{c}}{\mathbf{c}\cdot\mathbf{c}}, \frac{2\mathbf{a}\cdot\mathbf{b}}{\mathbf{c}\cdot\mathbf{c}}\right] \qquad (9.3.2.1)$$

provided that the vectors **a**, **b**, **c** describe the Niggli cell of L and fulfil the conditions (9.2.2.2*a*) to (9.2.2.5*f*) of Section 9.2.2. If $\mathscr{L}$ is a set of lattices then the set of Niggli points of all lattices of $\mathscr{L}$ is called the *Niggli image* of $\mathscr{L}$.

Thus we can speak about the Niggli image of a Bravais type $\mathscr{T}$. This Niggli image is a part of E_5 and so can be partitioned into components. This division of Niggli points induces back a division of lattices of the Bravais type $\mathscr{T}$. It turns out that this division is identical with the division of $\mathscr{T}$ into lattice characters as introduced in Section 9.2.5. This fact, used conversely, can be considered an exact definition of the lattice characters: Two lattices of Bravais type $\mathscr{T}$ are said to be of the same lattice character if their Niggli points lie in the same component of the Niggli image of $\mathscr{T}$.

We can, of course, also speak about Niggli images of particular lattice characters. According to their definition, these images are connected sets. However, much more can be stated about them: these sets are even *convex* (Fig. 9.3.2.2). This means that any two points of the Niggli image of a lattice character can be connected by a *straight segment* lying totally in this Niggli image. From this property, it follows that the lattice characters may be defined also in the following equivalent way:

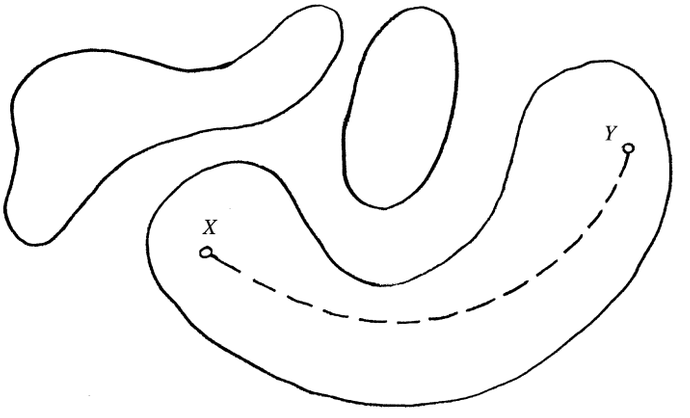

Fig. 9.3.2.1. A set $M \subset E_2$ consisting of three components.

* See, however, later parts of this section.
† Meaning that this cell has the smallest surface of all Buerger cells of the lattice.
‡ The deviation of a cell is the number $|90^\circ - \alpha| + |90^\circ - \beta| + |90^\circ - \gamma|$.
§ This cell need not be a Buerger cell.

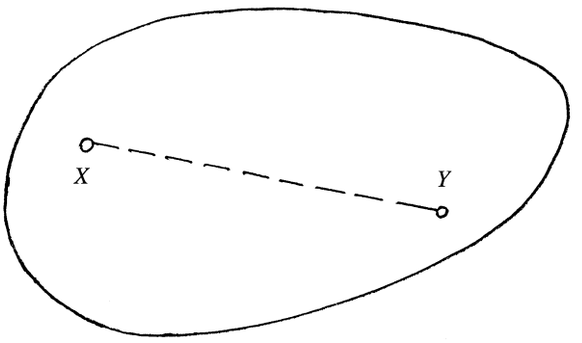

Fig. 9.3.2.2. A convex set in E_2.

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 **c** vector onto the **ab** plane provided the vectors **a**, **b**, **c** describe the Niggli cell of L and fulfil the conditions (9.2.2.2*a*) to (9.2.2.5*f*) 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, 1997*a*). 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

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

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 (**a**, **b**, **c**) in L such that

(i) the centring of (**a**, **b**, **c**) agrees with the centring mode given in column 2 in the *i*th entry, and

(ii) the parameters of the cell (**a**, **b**, **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 $\mathscr{T}$ into components. Doing

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 $k \leq 6$.

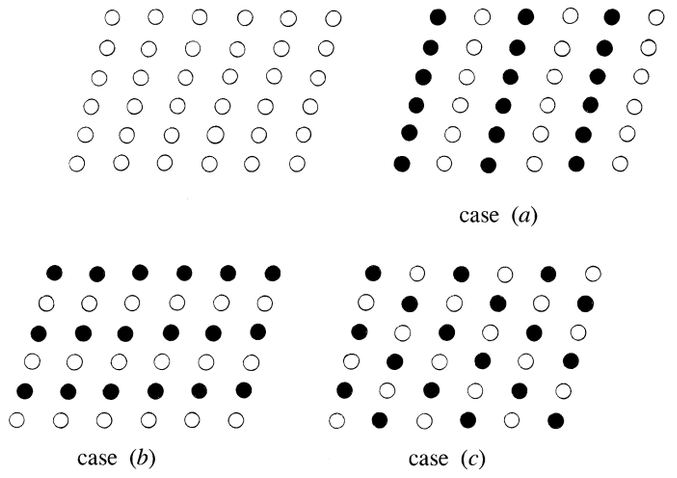

Fig. 9.3.6.1. Three possible decompositions of a two-dimensional lattice L into sublattices of index 2.

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.

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