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3.1. Crystal lattices

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3.1.1. Bases and lattices

By H. Burzlaff and H. Zimmermann

3.1.1.1. Description and transformation of bases

In three dimensions, a coordinate system is defined by an origin and a basis consisting of three non-coplanar vectors. The lengths a, b, c of the basis vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$ and the intervector angles $\alpha = \measuredangle(\mathbf{b}, \mathbf{c})$, $\beta = \measuredangle(\mathbf{c}, \mathbf{a})$, $\gamma = \measuredangle(\mathbf{a}, \mathbf{b})$ are called the *metric parameters*. In n dimensions, the lengths are designated a_i and the angles α_{ik}, where $1 \leq i < k \leq n$.

Another description of the basis consists of the scalar products of all pairs of basis vectors. The set of these scalar products obeys the rules of covariant tensors of the second rank (see Section 1.5.2). The scalar products may be written in the form of a (3×3) matrix

$$(\mathbf{a}_i \cdot \mathbf{a}_k) = (g_{ik}) = \boldsymbol{G}, \quad i, k = 1, 2, 3,$$

which is called the *matrix of the metric coefficients* or the *metric tensor*.

The change from one basis to another is described by a transformation matrix $\boldsymbol{P}$. The transformation of the old basis $(\mathbf{a}, \mathbf{b}, \mathbf{c})$ to the new basis $(\mathbf{a}', \mathbf{b}', \mathbf{c}')$ is given by

$$(\mathbf{a}', \mathbf{b}', \mathbf{c}') = (\mathbf{a}, \mathbf{b}, \mathbf{c}) \cdot \boldsymbol{P}. \tag{3.1.1.1}$$

The relation

$$\boldsymbol{G}' = \boldsymbol{P}^{\mathrm{T}} \cdot \boldsymbol{G} \cdot \boldsymbol{P} \tag{3.1.1.2}$$

holds for the metric tensors $\boldsymbol{G}$ and $\boldsymbol{G}'$.

3.1.1.2. Lattices

A three-dimensional lattice can be visualized best as an infinite periodic array of points, which are the termini of the vectors

$$\mathbf{l}_{uvw} = u\mathbf{a} + v\mathbf{b} + w\mathbf{c}, \quad u, v, w \text{ all integers.}$$

The parallelepiped determined by the basis vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$ is called a (primitive) *unit cell* of the lattice (*cf.* Section 1.3.2.3), $\mathbf{a}, \mathbf{b}$ and $\mathbf{c}$ are a primitive *basis of the lattice*. The number of possible lattice bases is infinite.

For the investigation of the properties of lattices, appropriate bases are required. In order to select suitable bases (see below), transformations may be necessary (Chapter 1.5). Of the several properties of lattices, only symmetry and some topological aspects are considered in this section. Some further properties of lattices are given in Section 3.1.4.

3.1.1.3. Topological properties of lattices

The treatment of the topological properties is restricted here to the consideration of the neighbourhood of a lattice point. For this purpose, the *domain of influence* (*Wirkungsbereich*, Dirichlet domain, Voronoi domain, Wigner–Seitz cell) (Delaunay, 1933) is introduced. The domain of a particular lattice point consists of all points in space that are closer to this lattice point than to any other lattice point or at most equidistant to it. To construct the domain, the selected lattice point is connected to all other lattice points. The set of planes perpendicular to these connecting lines and passing through their midpoints contains the boundary planes of the domain of influence, which is thus a convex polyhedron. (Niggli and Delaunay used the term 'domain of influence' for the interior of the convex polyhedron only.) Without the use of metrical properties, Minkowski (1897) proved that the maximal number of boundary planes resulting from this construction is equal to $2(2^n - 1)$, where n is the dimension of the space. The minimal number of boundary planes is $2n$. Each face of the polyhedron represents a lattice vector. Thus, the topological, metrical and symmetry properties of infinite lattices can be discussed with the aid of a single finite polyhedron, namely the domain of influence (*cf.* Burzlaff & Zimmermann, 1977).

3.1.1.4. Special bases for lattices

Different procedures are in use to select special bases of lattices. The reduction procedures employ metrical properties to develop a sequence of basis transformations which lead to a *reduced basis* and *reduced cell* (see Section 3.1.4).

Another possibility is to make use of the symmetry properties of lattices. This procedure, with the additional aid of standardization rules, leads to the *conventional crystallographic basis* and *cell*. In addition to translational symmetry, a lattice possesses point-group symmetry. No crystal can have higher point-group symmetry than the point group of its lattice, which is called its *holohedry*. (Detailed treatment of the symmetry properties of lattices and their classification is given in Chapter 1.3. Following the terminology introduced there, the lattice point groups are the geometric classes to which the Bravais groups of the lattices belong.) The seven holohedries in three dimensions and the four in two dimensions form the basis for the classification of lattices (Table 3.1.1.1). It may be shown by an algebraic approach (Burckhardt, 1966) or a topological one (Delaunay, 1933) that the arrangement of the symmetry elements with respect to the lattice vectors is not arbitrary but well determined. Taking as basis vectors lattice vectors along important symmetry directions and choosing the origin in a lattice point simplifies the description of the lattice symmetry operations (*cf.* Section 3.3.1). Note that such a basis is not necessarily a (primitive) basis of the lattice (see below). The choice of a basis controlled by symmetry is not always unique; in the monoclinic system, for example, one vector can be taken parallel to the symmetry direction but the other two vectors, perpendicular to it, are not uniquely determined by symmetry.

The choice of conventions for standardizing the setting of a lattice depends on the purpose for which it is used. The several sets of conventions rest on two conflicting principles: symmetry considerations and metric considerations. The following rules (i) to (vii) defining a *conventional basis* are taken from Donnay (1943; Donnay & Ondik, 1973); they deal with the conventions based on symmetry:

(i) Each basis vector is a lattice vector from the origin to the nearest node on the related row. The basis must define a right-handed coordinate system.

Table 3.1.1.1
Lattice point-group symmetries

(*a*) Two dimensions.

Lattice point group	2	2*mm*	4*mm*	6*mm*
Crystal family†	*m*	*o*	*t*	*h*
	*m*onoclinic (oblique)	*o*rthorhombic (rectangular)	*t*etragonal (square)	*h*exagonal

(*b*) Three dimensions.

Lattice point group	$C_i \equiv \bar{1}$	$C_{2h} \equiv 2/m$	$D_{2h} \equiv mmm$	$D_{4h} \equiv 4/mmm$	$D_{3d} \equiv \bar{3}m$	$D_{6h} \equiv 6/mmm$	$O_h \equiv m\bar{3}m$
Crystal family†	*a*	*m*	*o*	*t*	*h*		*c*
	*a*northic (triclinic)	*m*onoclinic	*o*rthorhombic	*t*etragonal	*h*exagonal		*c*ubic

† The symbols for crystal families were adopted by the International Union of Crystallography in 1985; *cf.* de Wolff *et al.* (1985).

(ii) The basis vectors for a *cubic* lattice are parallel to the fourfold axes.

(iii*a*) In a *hexagonal* lattice, the basis vector parallel to the sixfold axis is labelled **c**. The remaining two basis vectors are taken along equivalent twofold axes and they must include an angle of 120°; from the two possible sets, the shorter vectors are chosen.

(iii*b*) For *rhombohedral* lattices, two descriptions are given in the present edition, as in earlier ones. The first description which results in the conventional cell uses 'hexagonal axes'. In this case, **c** is taken along the threefold axis. The remaining two vectors are chosen along equivalent twofold axes, which include an angle of 120°; they are oriented so that lattice points occur at $2/3, 1/3, 1/3$ and $1/3, 2/3, 2/3$ (obverse setting). The reverse setting ($0, 0, 0$; $1/3, 2/3, 1/3$; $2/3, 1/3, 2/3$) is not used in the space-group tables (*cf.* the second footnote to Table 2.1.1.2). The second description uses 'rhombohedral axes': **a**, **b** and **c** are the shortest three non-coplanar lattice vectors symmetry-equivalent with respect to the threefold axis.

(iv) In a *tetragonal* lattice, the vector **c** is along the fourfold axis, and **a** and **b** are chosen along equivalent twofold axes perpendicular to each other. From the two possible sets, the shorter vectors are chosen.

(v) In an *orthorhombic* lattice, **a**, **b** and **c** must be taken along the three twofold axes.

(vi) For *monoclinic* lattices, two 'settings' are given in the present edition. In one setting, the only symmetry direction is labelled **b** (*b*-unique setting). The basis vectors **a** and **c** are chosen to be the shortest two vectors in the net plane perpendicular to **b**, the angle β should be non-acute. This occurs if

$$0 \leq -2\mathbf{a} \cdot \mathbf{c} \leq \min(a^2, c^2). \qquad (3.1.1.3)$$

In the other setting, the symmetry direction is labelled **c** [*c*-unique setting; first introduced in *International Tables for X-ray Crystallography* (1952)]. In this case, **a** and **b** are the shortest two vectors in the net plane perpendicular to **c** and the angle γ should be non-acute. The *b*-unique setting is considered to be the standard setting.

(vii) The reduced basis is used to describe a *triclinic* (= *anorthic*) lattice (*cf.* Section 3.1.4).

The metric parameters of the conventional basis are called *lattice parameters*. For the purpose of identification, additional metric rules are to be applied to make the labelling unique; they can be found in the introduction to *Crystal Data* (Donnay & Ondik, 1973).

When the above rules have been applied, it may occur that not all lattice points can be described by integral coordinates. In such cases, the unit cell contains two, three or four lattice points. The additional points may be regarded as *centrings* of the conventional cell. They have simple rational coordinates. For a conventional basis, the number of lattice points per cell is 1, 2, 3 or 4 (see Tables 3.1.2.1 and 3.1.2.2).

In two dimensions, only two centring types are needed:

p: no centring (primitive);
c: face centred.

In three dimensions, the following centring types are used:

P: no centring (primitive);
I: body centred (*innenzentriert*);
F: all-face centred;
A, *B*, *C*: one-face centred, either (**b**, **c**) or (**c**, **a**) or (**a**, **b**);
R: hexagonal cell rhombohedrally centred [see rule (iii*b*) above].

In orthorhombic and monoclinic lattices, some differently centred cells can be transformed into each other without violating the symmetry conditions for the choice of the basis vectors. In these cases, the different centred cells belong to the same *centring mode*. In the orthorhombic case, the three types of one-face-centred cells belong to the same centring mode because the symbol of the cell depends only on the labelling of the basis vectors; *C* is usually preferred to *A* and *B* as the standard setting; the centring mode is designated *S* (*seitenflächenzentriert*). In the monoclinic case (*b*-unique setting), *A*, *I* and *C* may occur if the basis is chosen according to rule (vi). They can be transformed into each other without changing the symmetry direction. *C* is used for the standard setting (*cf.* Section 2.1.1.2); it represents the centring mode *S*. The vectors **a**, **c** are conventionally chosen as short as the *C*-centring allows so that they need not be the shortest two vectors in their net plane and need not fulfil the inequalities (3.1.1.3).

3.1.1.5. Remarks

(i) For the handling of special problems such as subgroup relations, it may be convenient to use additional types of centred cells, *e.g.* a hexagonal cell centred at $2/3, 1/3, 0$ and $1/3, 2/3, 0$, which is called *H*. In this case, rule (iii*a*) above is violated as vectors **a** and **b** are now directed along the second set of equivalent twofold axes. Similarly, for tetragonal

lattices, *C* may be used instead of *P*, or *F* instead of *I*; *cf.* Sections 1.5.4 and 2.1.1.2.

(ii) Readers who have studied Chapter 1.3 may realize that the 'lattice bases' defined here are also called 'primitive bases' and that both 'primitive bases' and 'conventional bases' are special cases of bases used in crystallography.

3.1.2. Bravais types of lattices and other classifications

By H. Burzlaff and H. Zimmermann

3.1.2.1. Classifications

By means of the above-mentioned lattice properties, it is possible to classify lattices according to various criteria. Lattices can be subdivided with respect to their topological types of domains, resulting in two classes in two dimensions and five classes in three dimensions. They are called *Voronoi types*. If the classification involves topological *and* symmetry properties of the domains, 24 *Symmetrische Sorten* (Delaunay, 1933) are obtained in three dimensions and 5 in two dimensions. Other classifications consider either the centring type or the point group of the lattice.

The most important classification takes into account both the lattice point-group symmetry and the centring mode (Bravais, 1866). The resulting classes are called *Bravais types of lattices* or, for short, *Bravais lattices*. Two lattices belong to the same Bravais type if and only if they coincide both in their point-group symmetry and in the centring mode of their conventional cells. The Bravais lattice characterizes the translational subgroup of a space group. The number of Bravais lattices is 1 in one dimension, 5 in two dimensions, 14 in three dimensions and 64 in four dimensions. The Bravais lattices may be derived by topological (Delaunay, 1933) or algebraic procedures (Burckhardt, 1966; Neubüser *et al.*, 1971). It can be shown (Wondratschek *et al.*, 1971) that 'all Bravais types of the same [crystal] family can be obtained from each other by the process of centring'. As a consequence, different Bravais types of the same crystal family (*cf.* Section 1.3.4) differ in their centring mode. Thus, the Bravais types may be described by a lower-case letter designating the crystal family and an upper-case letter designating the centring mode. The relations between the point groups of the lattices and the crystal families are shown in Table 3.1.1.1. Since the hexagonal and rhombohedral Bravais types belong to the same crystal family, the rhombohedral lattice is described by *hR*, *h* indicating the family and *R* the centring type. This nomenclature was adopted for the 1969 reprint of *International Tables for X-ray Crystallography* (1952) and for *Structure Reports* since 1975 (*cf.* Trotter, 1975).

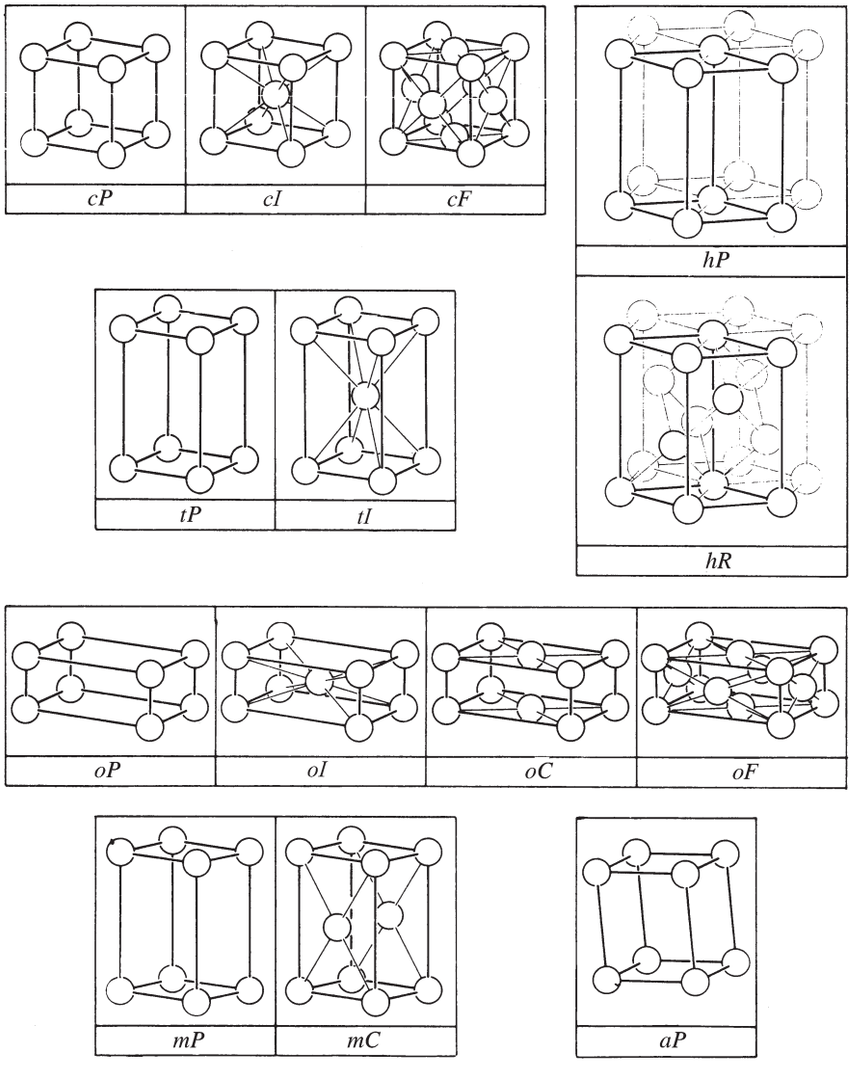


Figure 3.1.2.1
Conventional cells of the three-dimensional Bravais types of lattices (for symbols see Table 3.1.2.2).

3.1.2.2. Description of Bravais types of lattices

In Fig. 3.1.2.1, conventional cells for the 14 three-dimensional Bravais types of lattices are illustrated.

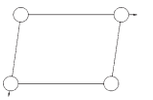
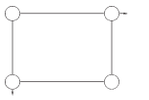
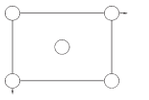
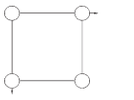
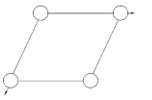
In Tables 3.1.2.1 and 3.1.2.2, the two- and three-dimensional Bravais types of lattices are described in detail. For each entry, the tables contain conditions that must be fulfilled by the lattice parameters and the metric tensor. These conditions are given with respect to two different basis systems, first the conventional basis related to symmetry, second a special primitive basis (see below). In columns 2 and 3, basis vectors not required by symmetry to be of the same length are designated by different letters. Columns 4 and 5 contain the metric tensors for the two related bases. Column 6 shows the relations between the components of the two tensors.

The last columns of Tables 3.1.2.1 and 3.1.2.2 show parallel projections of the appropriate conventional unit cells. Among the different possible choices of the primitive basis, as discussed in Section 3.1.1, the special primitive basis mentioned above is obtained according to the following rules:

(i) For each type of centring, only one transformation matrix $\boldsymbol{P}$ is used to obtain the primitive cell as given in Tables 3.1.2.1 and 3.1.2.2. The transformation obeys equation (3.1.1.2).

(ii) Among the different possible transformations, those are preferred which result in a metric tensor with simple relations among its components, as defined in Tables 3.1.2.1 and 3.1.2.2.

Table 3.1.2.1
Two-dimensional Bravais types of lattices

Bravais type of lattice†	Lattice parameters		Metric tensor			Projections
	Conventional	Primitive	Conventional	Primitive/ transformation to primitive cell	Relations of the components	
mp	a, b γ	a, b γ	$g_{11}\ \ g_{12}$ $\ \ \ g_{22}$	$g_{11}\ \ g_{12}$ $\ \ \ g_{22}$		
op	a, b $\gamma = 90°$	a, b $\gamma = 90°$	$g_{11}\ \ 0$ $\ \ \ g_{22}$	$g_{11}\ \ 0$ $\ \ \ g_{22}$		
oc		$a_1 = a_2, \gamma$		$\boldsymbol{P}(c)$‡ $g'_{11}\ \ g'_{12}$ $\ \ \ g'_{11}$	$g'_{11} = \frac{1}{4}(g_{11} + g_{22})$ $g'_{12} = \frac{1}{4}(g_{11} - g_{22})$ $g_{11} = 2(g'_{11} + g'_{12})$ $g_{12} = 2(g'_{11} - g'_{12})$	
tp	$a_1 = a_2$ $\gamma = 90°$	$a_1 = a_2$ $\gamma = 90°$	$g_{11}\ \ 0$ $\ \ \ g_{11}$	$g_{11}\ \ 0$ $\ \ \ g_{11}$		
hp	$a_1 = a_2$ $\gamma = 120°$	$a_1 = a_2$ $\gamma = 120°$	$g_{11}\ \ -\frac{1}{2}g_{11}$ $\ \ \ g_{11}$	$g_{11}\ \ -\frac{1}{2}g_{11}$ $\ \ \ g_{11}$		

† The symbols for Bravais types of lattices were adopted by the International Union of Crystallography in 1985; *cf.* de Wolff *et al.* (1985). ‡ $\boldsymbol{P}(c) = \frac{1}{2}(11/\bar{1}1)$.

If a primitive basis is chosen according to these rules, basis vectors of the conventional cell have parallel face-diagonal or body-diagonal orientation with respect to the basis vectors of the primitive cell. For cubic and rhombohedral lattices, the primitive basis vectors are selected such that they are symmetry-equivalent with respect to a threefold axis. In all cases, a face of the 'domain of influence' is perpendicular to each basis vector of these primitive cells.

3.1.2.3. Delaunay reduction and standardization

Further classifications use reduction theory. There are different approaches to the reduction of quadratic forms in mathematics. The two most important in our context are

(i) the Selling–Delaunay reduction (Selling, 1874),

(ii) the Eisenstein–Niggli reduction.

The investigations by Gruber (*cf.* Section 3.1.4) have shown the common root of both crystallographic approaches. As the Niggli reduction will be discussed in detail in Sections 3.1.3 and 3.1.4, we shall discuss the Delaunay reduction here.

We start with a lattice basis $(\mathbf{b}_i)_{1\le i\le n}$ $(n = 2, 3)$. This basis is extended by a vector

$$\mathbf{b}_{n+1} = -(\mathbf{b}_1 + \ldots + \mathbf{b}_n).$$

All scalar products

$$\mathbf{b}_i \cdot \mathbf{b}_k \ (1 \le i < k \le n+1)$$

are considered. The reduction is performed minimizing the sum

$$\sum = \mathbf{b}_1{}^2 + \ldots + \mathbf{b}_{n+1}{}^2.$$

It can be shown that this sum can be reduced by a sequence of transformations as long as one of the scalar products is still positive. If *e.g.* the scalar product $\mathbf{b}_1 \cdot \mathbf{b}_2$ is still positive, a transformation can be applied such that the sum $\sum'$ of the transformed $\mathbf{b}'^2_i$ is smaller than $\sum$:

$$\mathbf{b}'_1 = -\mathbf{b}_1,\ \mathbf{b}'_2 = \mathbf{b}_2,\ \mathbf{b}'_3 = \mathbf{b}_1 + \mathbf{b}_3 \text{ and } \mathbf{b}'_4 = \mathbf{b}_1 + \mathbf{b}_4.$$

In the two-dimensional case, $\mathbf{b}'_3 = 2\mathbf{b}_1 + \mathbf{b}_3$ holds.

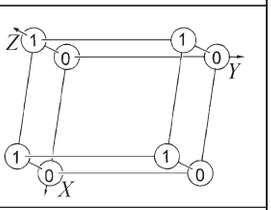
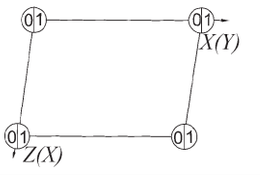
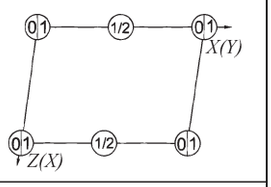
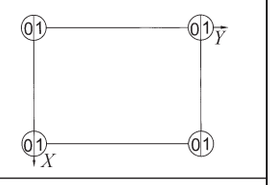
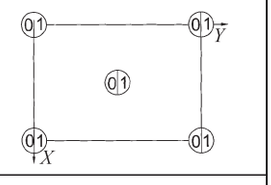
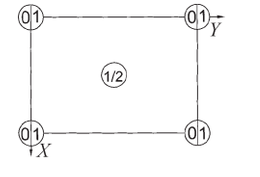
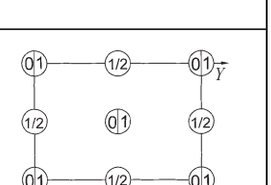
If all the scalar products are less than or equal to zero, the three shortest vectors of the reduced basis are contained in the set $\{\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3, \mathbf{b}_4, \mathbf{b}_1 + \mathbf{b}_2, \mathbf{b}_2 + \mathbf{b}_3, \mathbf{b}_3 + \mathbf{b}_1\}$, called the *Delaunay set*, which corresponds to the maximal set of faces of the Dirichlet domain (at most 14 faces).

The result of a reduction can be presented by a graphical symbol, the Selling tetrahedron. The four corners of the tetrahedron correspond to the vectors $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3, \mathbf{b}_4$, the mutual scalar products are attached to the edges. A scalar product that is zero is indicated by '0'; equal scalar products are designated by the same graphical symbol (*cf.* Table 3.1.2.3).

Delaunay's classification is based on Voronoi types. Voronoi distinguishes five classes of Dirichlet domains. To describe these, the following symbols are used to represent particular topological features: s is used for a hexagon and for v for a quadrangle, s^2 indicates an edge between two hexagons and v^2 an edge between two quadrangles, v^4 is a vertex where four quadrangles meet and v^3 is a vertex where three quadrangles meet. The five types are topologically characterized by: V1 ($8s$, $6v$, $12s^2$), V2 ($4s$, $8v$, $4s^2$), V3 ($12v$, $24v^2$, $8v^3$, $6v^4$), V4 ($2s$, $6v$, $6v^2$) and V5 ($6v$, $12v^2$, $8v^3$). The numbers give the multiplicities of each feature.

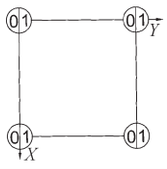
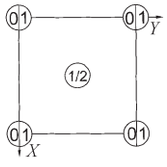
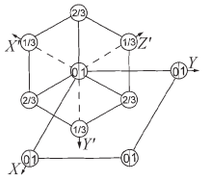
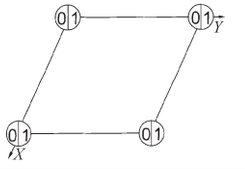
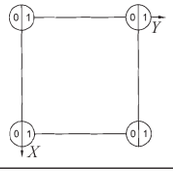
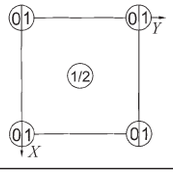
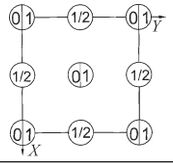
Delaunay combined the topological description with the rotation groups of the crystallographic holohedries. He used upper-case letters for these groups (K – cubic, H – hexagonal, R – rhombohedral, Q – tetragonal, O – orthorhombic, M – monoclinic, T – triclinic) followed by a incremental number if more than one Voronoi type with the same symmetry exists. The results are presented in Table 3.1.2.3. In each row a '*Symmetrische Sorte*' is described.

Table 3.1.2.2
Three-dimensional Bravais types of lattices

Bravais type of lattice†	Lattice parameters		Metric tensor			Projections
	Conventional	Primitive	Conventional	Primitive/transf.‡	Relations of the components	
aP	*a*, *b*, *c* α, β, γ	*a*, *b*, *c* α, β, γ	$g_{11}\ g_{12}\ g_{13}$ $g_{22}\ g_{23}$ g_{33}	$g_{11}\ g_{12}\ g_{13}$ $g_{22}\ g_{23}$ g_{33}		
mP	*a*, *b*, *c* β, $\alpha = \gamma = 90°$	*a*, *b*, *c* β, $\alpha = \gamma = 90°$	$g_{11}\ 0\ g_{13}$ $g_{22}\ 0$ g_{33}	$g_{11}\ 0\ g_{13}$ $g_{22}\ 0$ g_{33}		
mC (*mS*)		$a_1 = a_2$, *c* γ, $\alpha = \beta$		$\boldsymbol{P}(C)$ $g'_{11}\ g'_{12}\ g'_{13}$ $g'_{11}\ g'_{13}$ g_{33}	$g'_{11} = \frac{1}{4}(g_{11} + g_{22})$ $g'_{12} = \frac{1}{4}(g_{11} - g_{22})$ $g'_{13} = \frac{1}{2}g_{13}$ $g_{11} = 2(g'_{11} + g'_{12})$ $g_{22} = 2(g'_{11} - g'_{12})$ $g_{13} = 2g'_{13}$	
oP	*a*, *b*, *c* $\alpha = \beta = \gamma = 90°$	*a*, *b*, *c* $\alpha = \beta = \gamma = 90°$	$g_{11}\ 0\ 0$ $g_{22}\ 0$ g_{33}	$g_{11}\ 0\ 0$ $g_{22}\ 0$ g_{33}		
oC (*oS*)		$a_1 = a_2$, *c* γ, $\alpha = \beta = 90°$		$\boldsymbol{P}(C)$ $g'_{11}\ g'_{12}\ 0$ $g'_{11}\ 0$ g_{33}	$g'_{11} = \frac{1}{4}(g_{11} + g_{22})$ $g'_{12} = \frac{1}{4}(g_{11} - g_{22})$ $g_{11} = 2(g'_{11} + g'_{12})$ $g_{22} = 2(g'_{11} - g'_{12})$	
oI		$a_1 = a_2 = a_3$ α, β, γ $\cos\alpha + \cos\beta + \cos\gamma = -1$		$\boldsymbol{P}(I)$ $-\tilde{g}\ g'_{12}\ g'_{13}$ $-\tilde{g}\ g'_{23}$ $-\tilde{g}$ $\tilde{g} = g'_{12} + g'_{13} + g'_{23}$	$g'_{12} = \frac{1}{4}(-g_{11} - g_{22} + g_{33})$ $g'_{13} = \frac{1}{4}(-g_{11} + g_{22} - g_{33})$ $g'_{23} = \frac{1}{4}(g_{11} - g_{22} - g_{33})$ $g_{11} = -2(g'_{12} + g'_{13})$ $g_{22} = -2(g'_{12} + g'_{23})$ $g_{33} = -2(g'_{13} + g'_{23})$	
oF		*a*, *b*, *c* α, β, γ $\cos\alpha = \dfrac{-a^2 + b^2 + c^2}{2bc}$ $\cos\beta = \dfrac{a^2 + b^2 + c^2}{2ac}$ $\cos\gamma = \dfrac{a^2 + b^2 - c^2}{2ab}$		$\boldsymbol{P}(F)$ $\tilde{g}_1\ g'_{12}\ g'_{13}$ $\tilde{g}_2\ g'_{23}$ $\tilde{g}_3$ $\tilde{g}_1 = g'_{12} + g'_{13}$ $\tilde{g}_2 = g'_{12} + g'_{23}$ $\tilde{g}_3 = g'_{13} + g'_{23}$	$g'_{12} = \frac{1}{4}g_{33}$ $g'_{13} = \frac{1}{4}g_{22}$ $g'_{23} = \frac{1}{4}g_{11}$ $g_{11} = 4g'_{23}$ $g_{22} = 4g'_{13}$ $g_{33} = 4g'_{12}$	

Column 1 contains the Delaunay description followed by the Voronoi type. Beneath these, the Bravais lattice and the symbol of its holohedry are given. Next the topological features that are compatible with the symmetry axes referred to the '*blickrichtungen*' of the holohedry are listed. Column 2 gives the metric conditions for the occurrence of certain Voronoi types. For the monoclinic cases with centred cells (*M*1–*M*5) it is useful to introduce in addition to the vectors **a**, **c**, **f** = **a** + **c** special parameters (p^2, q^2, r^2). **p** designates the vector below the centring point in the projection in the net perpendicular to **b**. **q** is the

Table 3.1.2.2 (continued)

Bravais type of lattice†	Lattice parameters		Metric tensor			Projections
	Conventional	Primitive	Conventional	Primitive/transf.‡	Relations of the components	
tP	$a_1 = a_2$, c $\alpha = \beta = \gamma = 90°$	$a_1 = a_2$, c $\alpha = \beta = \gamma = 90°$	$\begin{matrix} g_{11} & 0 & 0 \\ & g_{11} & 0 \\ & & g_{33} \end{matrix}$	$\begin{matrix} g_{11} & 0 & 0 \\ & g_{11} & 0 \\ & & g_{33} \end{matrix}$		
tI		$a_1 = a_2 = a_3$ $\gamma, \alpha = \beta$ $2\cos\alpha + \cos\gamma = -1$		$\boldsymbol{P}(I)$ $\begin{matrix} \bar{g} & g'_{12} & g'_{13} \\ & \bar{g} & g'_{13} \\ & & \bar{g} \end{matrix}$ $\bar{g} = -(g'_{12} + 2g'_{13})$	$g'_{12} = \frac{1}{4}(-2g_{11} + g_{33})$ $g'_{13} = -\frac{1}{4}g_{33}$ $g_{11} = 2(g'_{12} + g'_{13})$ $g_{33} = -4g'_{13}$	
hR	$a_1 = a_2$, c $\alpha = \beta = 90°$ $\gamma = 120°$	$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma$	$\begin{matrix} g_{11} & -\frac{1}{2}g_{11} & 0 \\ & g_{11} & 0 \\ & & g_{33} \end{matrix}$	$\boldsymbol{P}(R)$ $\begin{matrix} g'_{11} & g'_{12} & g'_{12} \\ & g'_{11} & g'_{12} \\ & & g'_{11} \end{matrix}$	$g'_{11} = \frac{1}{9}(3g_{11} + g_{33})$ $g'_{12} = \frac{1}{9}(-\frac{3}{2}g_{11} + g_{33})$ $g_{11} = 2(g'_{11} - g'_{12})$ $g_{33} = 3(g'_{11} + 2g'_{12})$	
hP		$a_1 = a_2$, c $\alpha = \beta = 90°$ $\gamma = 120°$		$\begin{matrix} g_{11} & -\frac{1}{2}g_{11} & 0 \\ & g_{11} & 0 \\ & & g_{33} \end{matrix}$		
cP	$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma = 90°$	$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma = 90°$	$\begin{matrix} g_{11} & 0 & 0 \\ & g_{11} & 0 \\ & & g_{11} \end{matrix}$	$\begin{matrix} g_{11} & 0 & 0 \\ & g_{11} & 0 \\ & & g_{11} \end{matrix}$		
cI		$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma = 109.5°$ $\cos\alpha = -\frac{1}{3}$		$\boldsymbol{P}(I)$ $\begin{matrix} g'_{11} & -\frac{1}{3}g'_{11} & -\frac{1}{3}g'_{11} \\ & g'_{11} & -\frac{1}{3}g'_{11} \\ & & g'_{11} \end{matrix}$	$g'_{11} = \frac{3}{4}g_{11}$ $g_{11} = \frac{4}{3}g'_{11}$	
cF		$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma = 60°$		$\boldsymbol{P}(F)$ $\begin{matrix} g'_{11} & \frac{1}{2}g'_{11} & \frac{1}{2}g'_{11} \\ & g'_{11} & \frac{1}{2}g'_{11} \\ & & g'_{11} \end{matrix}$	$g'_{11} = \frac{1}{2}g_{11}$ $g_{11} = 2g'_{11}$	

† The symbols for Bravais types of lattices were adopted by the International Union of Crystallography in 1985; *cf.* de Wolff *et al.* (1985). Symbols in parentheses are standard symbols, see Table 2.1.1.1. ‡ $\boldsymbol{P}(C) = \frac{1}{2}(110/\bar{1}10/002)$, $\boldsymbol{P}(I) = \frac{1}{2}(\bar{1}11/1\bar{1}1/11\bar{1})$, $\boldsymbol{P}(F) = \frac{1}{2}(011/101/110)$, $\boldsymbol{P}(R) = \frac{1}{3}(\bar{1}21/\bar{2}11/111)$.

shorter one of the other two vectors and **r** labels the remaining one (*cf.* Burzlaff & Zimmermann, 1985).

For practical applications, it is useful to classify the patterns of the resulting six scalar products regarding their equivalence or zero values in the form of a symbolic (Selling) tetrahedron (column 3). These classes of patterns correspond to the reduced bases. They result in 24 '*Symmetrische Sorten*' (Delaunay, 1933) that fix the Voronoi types and the holohedries, and simultaneously lead directly to the conventional crystallographic cells by fixed transformations (*cf.* Patterson & Love, 1957; Burzlaff & Zimmermann, 1993).

Column 4 contains projections of the Dirichlet domain along the symmetry directions indicated by the topological/symmetry symbol in column 1. Column 5 shows the relation between the Dirichlet domain and the conventional cell. Column 6 contains the transformation matrix from the reduced basis to the conventional basis. (*Note*: In the monoclinic centred case it leads to the *I* centring.)

Table 3.1.2.3
Delaunay types of lattices (‘*Symmetrische Sorten*’)

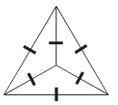
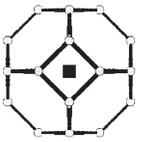
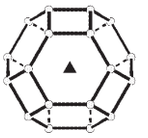
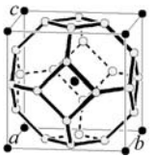
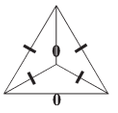
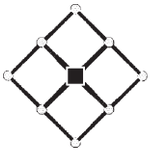
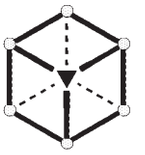
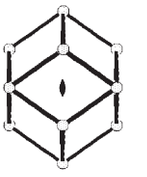
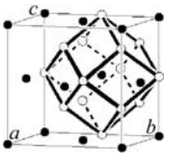
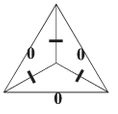
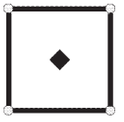
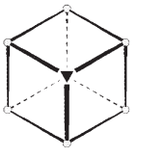
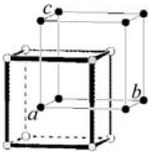
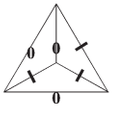
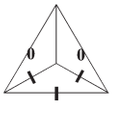
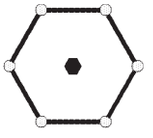
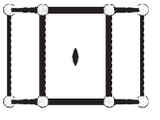
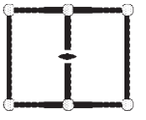
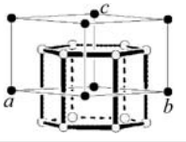
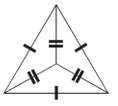
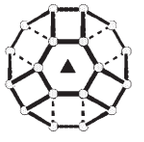
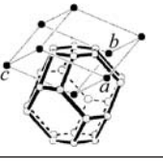
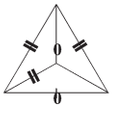
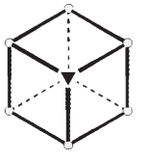
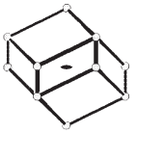
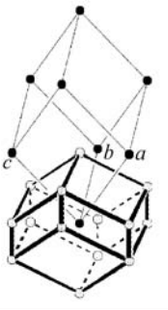
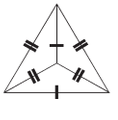
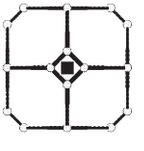
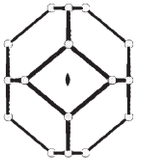
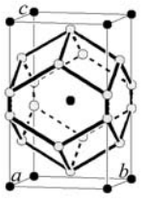
Delaunay–Voronoi type	Metric conditions	Selling tetrahedron	Projections along symmetry directions			Dirichlet domain in the unit cell	Transformation to the conventional cell
*K*1 V1 *cI* $\frac{4}{m}\bar{3}\frac{2}{m}$ *v s* s^2	–						$\begin{pmatrix}0&1&1\\1&0&1\\1&1&0\end{pmatrix}$
*K*2 V3 *cF* $\frac{4}{m}\bar{3}\frac{2}{m}$ v^4 v^3 *v*	–						$\begin{pmatrix}1&-1&1\\1&1&1\\0&0&2\end{pmatrix}$
*K*3 V5 *cP* $\frac{4}{m}\bar{3}\frac{2}{m}$ *v* v^3 v^2	–						$\begin{pmatrix}1&0&0\\0&0&1\\0&1&1\end{pmatrix}$
							$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$
H V4 *hP* $\frac{6}{m}\frac{2}{m}\frac{2}{m}$ *s v* v^2	–						$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$
*R*1 V1 *hR* $\bar{3}\frac{2}{m}$ *s* s^2	$2c^2 < 3a^2$				–		$\begin{pmatrix}1&0&1\\-1&1&1\\0&-1&1\end{pmatrix}$
*R*2 V3 *hR* $\bar{3}\frac{2}{m}$ v^3 *v*	$2c^2 > 3a^2$				–		$\begin{pmatrix}1&0&1\\0&0&3\\0&1&2\end{pmatrix}$
*Q*1 V1 *tI* $\frac{4}{m}\frac{2}{m}\frac{2}{m}$ *v v* s^2	$c^2 < 2a^2$						$\begin{pmatrix}0&1&1\\1&0&1\\1&1&0\end{pmatrix}$

Table 3.1.2.3 (continued)

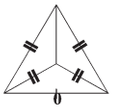
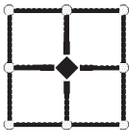
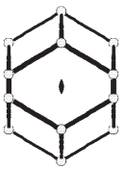
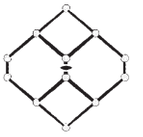
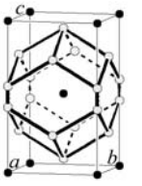
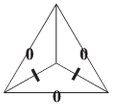
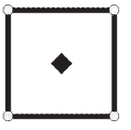
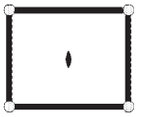
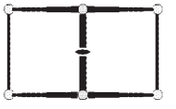
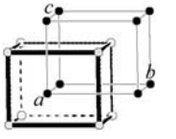
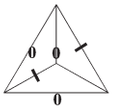
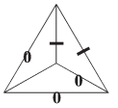
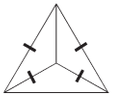
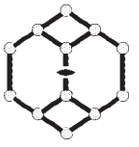
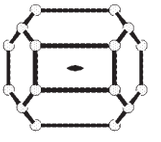
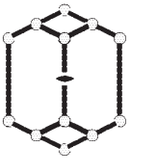
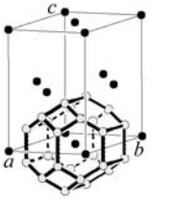
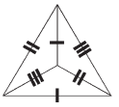
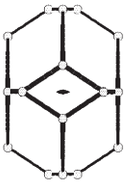
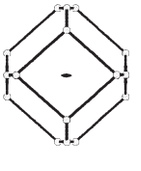
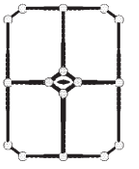
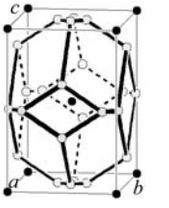
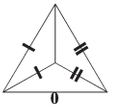
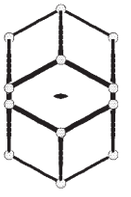
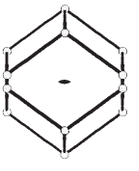
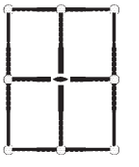
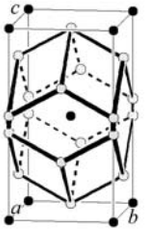
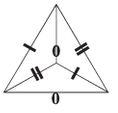
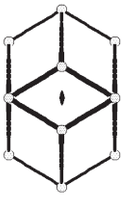
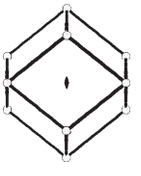
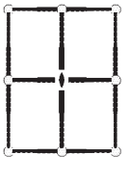
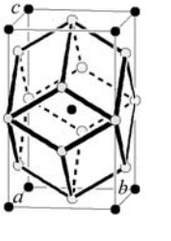
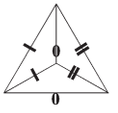
Delaunay–Voronoi type	Metric conditions	Selling tetrahedron	Projections along symmetry directions			Dirichlet domain in the unit cell	Transformation to the conventional cell
$Q2$ V2 tI $\frac{4}{m}\frac{2}{m}\frac{2}{m}$ $v^4\ s\ s^2$	$c^2 > 2a^2$						$\begin{pmatrix}1&0&1\\0&1&1\\0&0&2\end{pmatrix}$
$Q3$ V5 tP $\frac{4}{m}\frac{2}{m}\frac{2}{m}$ $v\ v\ v^2$	–						$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$
							$\begin{pmatrix}1&0&0\\0&0&1\\0&1&1\end{pmatrix}$
							$\begin{pmatrix}0&0&1\\1&1&0\\0&1&0\end{pmatrix}$
$O1$ V1 oF $\frac{2}{m}\frac{2}{m}\frac{2}{m}$ $s^2\ v\ s^2$	–						$\begin{pmatrix}1&-1&1\\1&1&1\\0&0&2\end{pmatrix}$
$O2$ V1 oI $\frac{2}{m}\frac{2}{m}\frac{2}{m}$ $v\ v\ v$	$a^2 + b^2 > c^2$						$\begin{pmatrix}0&1&1\\1&0&1\\1&1&0\end{pmatrix}$
$O3$ V2 oI $\frac{2}{m}\frac{2}{m}\frac{2}{m}$ $s\ s\ v^4$	$a^2 + b^2 < c^2$						$\begin{pmatrix}1&0&1\\0&1&1\\0&0&2\end{pmatrix}$
$O4$ V3 oI $\frac{2}{m}\frac{2}{m}\frac{2}{m}$ $v\ v\ v^4$	$a^2 + b^2 = c^2$						$\begin{pmatrix}0&1&1\\1&0&1\\1&1&0\end{pmatrix}$
							$\begin{pmatrix}1&0&1\\0&1&1\\0&0&2\end{pmatrix}$

Table 3.1.2.3 (continued)

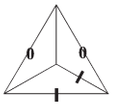
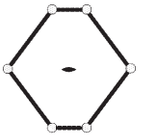
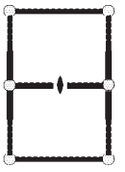
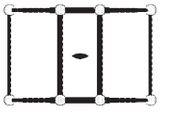
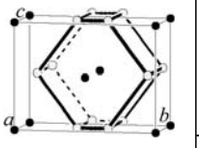
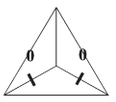
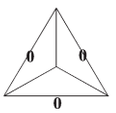
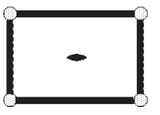
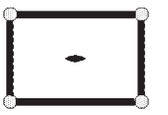
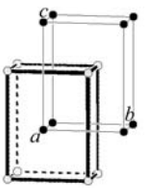
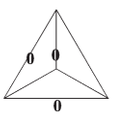
Delaunay–Voronoi type	Metric conditions	Selling tetrahedron	Projections along symmetry directions			Dirichlet domain in the unit cell	Transformation to the conventional cell
*O*5 V4 *o*(*AB*)*C* $\frac{2}{m}\frac{2}{m}\frac{2}{m}$ *s* v^2 *v*	–						$\begin{pmatrix}2&0&0\\1&1&0\\0&0&1\end{pmatrix}$
							$\begin{pmatrix}1&1&0\\-1&1&0\\0&0&1\end{pmatrix}$
*O*6 V5 *oP* $\frac{2}{m}\frac{2}{m}\frac{2}{m}$ *v v v*	–						$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$
							$\begin{pmatrix}1&0&0\\0&0&1\\0&1&1\end{pmatrix}$

Table 3.1.2.3 (continued)

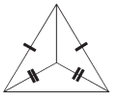
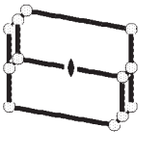
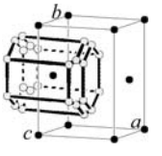
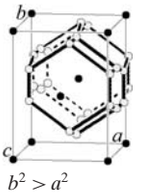
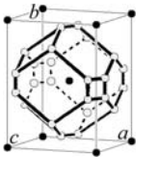
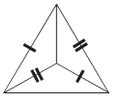
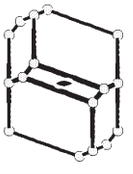
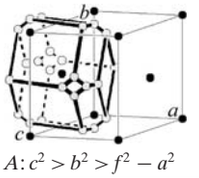
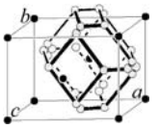
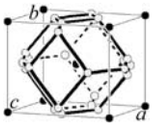
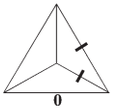
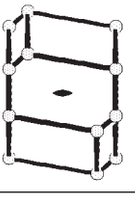
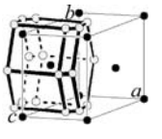
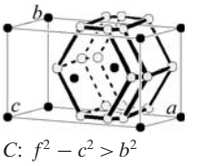
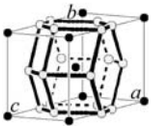
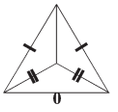
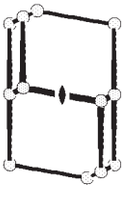
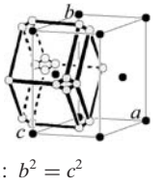
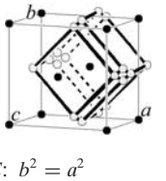
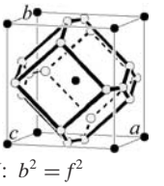
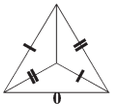
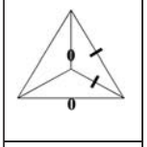
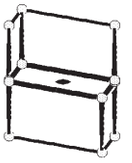
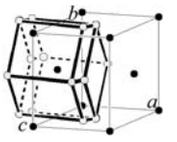
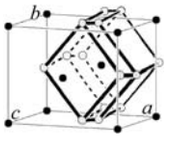
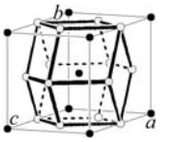
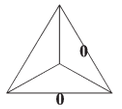
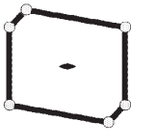
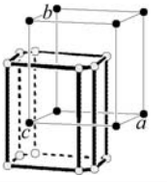
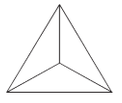
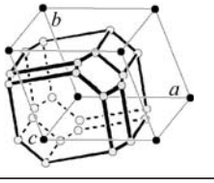
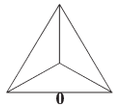
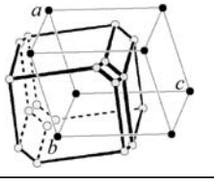
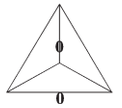
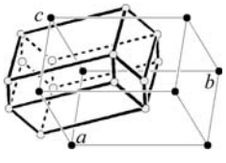
Delaunay–Voronoi type	Metric conditions	Selling tetrahedron	Projections along symmetry directions	Dirichlet domain in the unit cell			Transformation to the conventional cell
*M*1 V1 *m*(*AC*)*I* $\frac{2}{m}$ s^2	$b^2 > p^2$			 *A*: $b^2 > c^2$	 *C*: $b^2 > a^2$	 *I*: $b^2 > f^2$	$\begin{pmatrix}-1&1&0\\-1&-1&0\\-1&0&1\end{pmatrix}$
*M*2 V1 *m*(*AC*)*I* $\frac{2}{m}$ *v*	$p^2 > b^2$, $b^2 > r^2 - q^2$			 *A*: $c^2 > b^2 > f^2 - a^2$	 *C*: $a^2 > b^2 > f^2 - c^2$	 *I*: $f^2 > b^2 > c^2 - a^2$	$\begin{pmatrix}0&1&-1\\1&1&0\\1&0&-1\end{pmatrix}$
*M*3 V2 *m*(*AC*)*I* $\frac{2}{m}$ *s*	$r^2 - q^2 > b^2$			 *A*: $f^2 - a^2 > b^2$	 *C*: $f^2 - c^2 > b^2$	 *I*: $c^2 - a^2 > b^2$	$\begin{pmatrix}-1&0&1\\-1&1&0\\-2&0&0\end{pmatrix}$
*M*4 V4 *m*(*AC*)*I* $\frac{2}{m}$ s^2	$b^2 = p^2$			 *A*: $b^2 = c^2$	 *C*: $b^2 = a^2$	 *I*: $b^2 = f^2$	$\begin{pmatrix}0&1&-1\\1&1&0\\1&0&-1\end{pmatrix}$
							$\begin{pmatrix}-1&1&0\\-1&-1&0\\-1&0&1\end{pmatrix}$

Table 3.1.2.3 (continued)

Delaunay–Voronoi type	Metric conditions	Selling tetrahedron	Projections along symmetry directions	Dirichlet domain in the unit cell	Transformation to the conventional cell
*M*5 V3 *m*(*AC*)*I* $\frac{2}{m}$ *v*	$b^2 = r^2 - q^2$			 *A*: $b^2 = f^2 - a^2$  *C*: $b^2 = f^2 - c^2$  *I*: $b^2 = c^2 - a^2$	$\begin{pmatrix} -1 & 0 & 1 \\ -1 & 1 & 0 \\ -2 & 0 & 0 \end{pmatrix}$ $\begin{pmatrix} 1 & 0 & -1 \\ 1 & -1 & 0 \\ 0 & -1 & -1 \end{pmatrix}$
*M*6 V4 *mP* $\frac{2}{m}$ *s*	–				$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
*T*1 V1 *aP* 1	–				$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
*T*2 V2 *aP* 1	$\mathbf{a} \cdot \mathbf{b} = 0$				$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
*T*3 V3 *aP* 1	$\mathbf{a} \cdot \mathbf{b} = 0$ $(\mathbf{a} + \mathbf{b} + \mathbf{c}) \cdot \mathbf{c} = 0$				$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

In some cases, different Selling patterns are given for one '*Symmetrische Sorte*'. This procedure avoids a final reduction step (*cf.* Patterson & Love, 1957) and simplifies the computational treatment significantly. The number of '*Symmetrische Sorten*', and thus the number of transformations which have to be applied, is smaller than the number of lattice characters according to Niggli. Note that the introduction of reduced bases using shortest lattice vectors causes complications in more than three dimensions (*cf.* Schwarzenberger, 1980).

3.1.2.4. Example of Delaunay reduction and standardization of the basis

Let the basis $\mathbf{B} = (\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3)$ given by the scalar products

$$\begin{pmatrix} g_{11} & g_{22} & g_{33} \\ g_{23} & g_{31} & g_{12} \end{pmatrix} = \begin{pmatrix} 6 & 8 & 8 \\ 4 & 2 & 3 \end{pmatrix}$$

or by $b_1 = 2.449$ ($\sqrt{6}$), $b_2 = b_3 = 2.828$ ($\sqrt{8}$) (in arbitrary units), $\beta_{23} = 60°$ ($\cos\beta_{23} = \frac{1}{2}$), $\beta_{13} = 73.22°$ ($\cos\beta_{13} = \sqrt{3}/6$), $\beta_{12} = 64.34°$ ($\cos\beta_{12} = \sqrt{3}/4$).

The aim is to find a standardized basis of shortest lattice vectors using Delaunay reduction. This example, given by B. Gruber (*cf.* Burzlaff & Zimmermann, 1985), shows the standardization problems remaining after the reduction.

The general reduction step can be described using Selling four flats. The corners are designated by the vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}, \mathbf{d} = -\mathbf{a} - \mathbf{b} - \mathbf{c}$. The edges are marked by the scalar products among these vectors. If positive scalar products can be found, choose the largest: $\mathbf{a} \cdot \mathbf{b}$ (indicated as **ab** in Fig. 3.1.2.2*a*). The reduction transformation is: $\mathbf{a}_D = \mathbf{a}$, $\mathbf{b}_D = -\mathbf{b}$, $\mathbf{c}_D = \mathbf{c} + \mathbf{b}$, $\mathbf{d}_D = \mathbf{d} + \mathbf{b}$ (see Fig. 3.1.2.2*a*). In this example, this results in the Selling four flat shown in Fig. 3.1.2.2(*b*). The next step, shown in Fig. 3.1.2.2(*c*), uses the (maximal) positive scalar product for further reduction. Finally, using $\mathbf{b}_2 + \mathbf{b}_3 + \mathbf{b}_4 = -\mathbf{b}_1$ we get the result shown in Fig. 3.1.2.2(*d*).

The complete procedure can be expressed in a table, as shown in Table 3.1.2.4. Each pair of lines contains the starting basis and

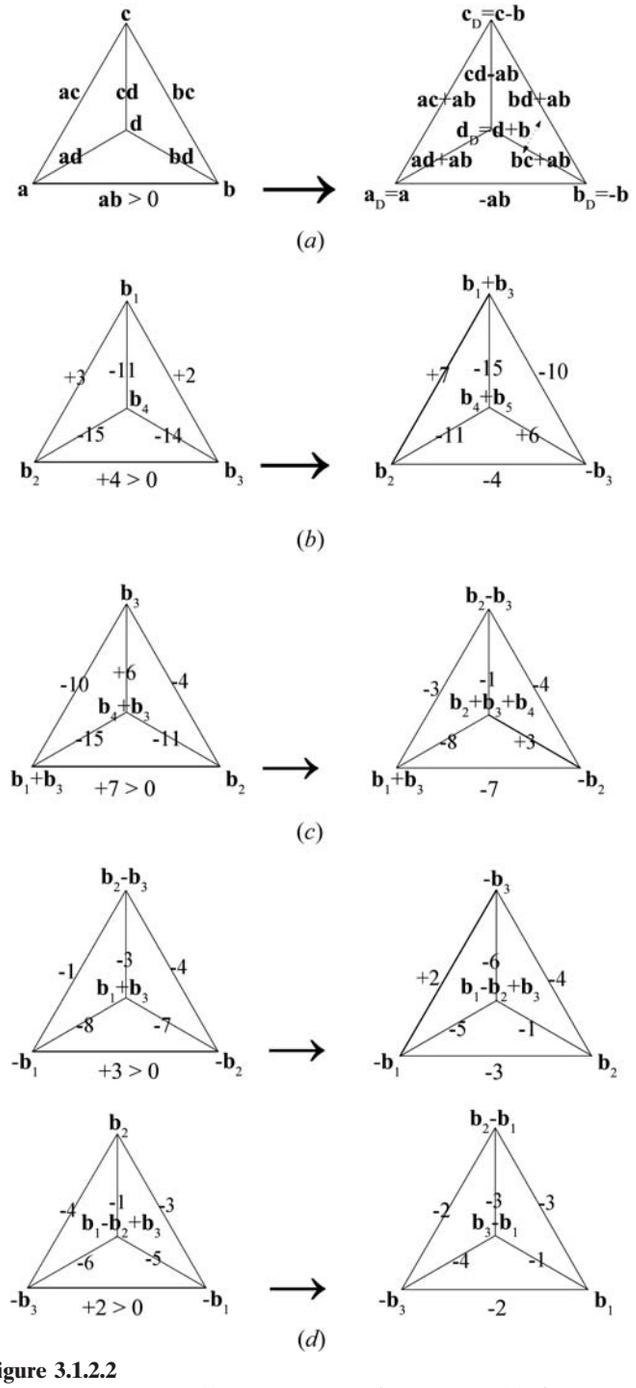


Figure 3.1.2.2
Delaunay reduction of Gruber's example (*cf.* Section 3.1.2.4). The edges of Selling tetrahedra are labelled by the scalar products of the vectors which designate the corners of the tetrahedra.

Table 3.1.2.5
Discussion of Gruber's example using the cell surface

No.	$(\mathbf{b}_1^s, \mathbf{b}_2^s, \mathbf{b}_3^s)$	Homogenous corner	Surface (surface units)
1	$(+\mathbf{b}_D, +\mathbf{a}_D, +\mathbf{c}_D)$	Non-acute	41.25
2	$(+\mathbf{b}_D, +\mathbf{a}_D, +\mathbf{d}_D)$	Non-acute	40.83
3	$(+\mathbf{b}_D, -\mathbf{a}_D, \mathbf{b}_D + \mathbf{c}_D)$	Acute	39.61
4	$(+\mathbf{b}_D, +\mathbf{c}_D, +\mathbf{d}_D)$	Non-acute	41.03
5	$(+\mathbf{b}_D, -\mathbf{d}_D, \mathbf{b}_D + \mathbf{c}_D)$	Acute	40.06

its scalar products before transformation as the first line, and then the transformed scalar products and the Delaunay basis after transformation below. In our case, four transformation steps are necessary. The result is

$$\mathbf{a}_D = -\mathbf{b}_3, \quad \mathbf{b}_D = \mathbf{b}_1, \quad \mathbf{c}_D = \mathbf{b}_2 - \mathbf{b}_1, \quad \mathbf{d}_D = \mathbf{b}_3 - \mathbf{b}_1.$$

The final Selling tetrahedron shows that the Dirichlet domain belongs to Voronoi type 1. It fulfils no symmetry condition and thus corresponds to an anorthic (triclinic) lattice.

For further standardization we consider the Delaunay set

$$\{\pm\mathbf{a}_D, \pm\mathbf{b}_D, \pm\mathbf{c}_D, \pm\mathbf{d}_D = -(\mathbf{a}_D + \mathbf{b}_D + \mathbf{c}_D), \pm(\mathbf{b}_D + \mathbf{c}_D), \pm(\mathbf{a}_D + \mathbf{c}_D), \pm(\mathbf{a}_D + \mathbf{b}_D)\}.$$

All bases of shortest lattice vectors $(\mathbf{b}_1^s, \mathbf{b}_2^s, \mathbf{b}_3^s)$ can be found:

$$|\mathbf{a}_D|^2 = 8, \quad |\mathbf{b}_D|^2 = 6, \quad |\mathbf{c}_D|^2 = 8, \quad |\mathbf{d}_D|^2 = 8,$$
$$|\mathbf{b}_D + \mathbf{c}_D|^2 = 8, \quad |\mathbf{a}_D + \mathbf{c}_D|^2 = 12, \quad |\mathbf{a}_D + \mathbf{b}_D|^2 = 10.$$

Any basis of shortest lattice vectors contains $\mathbf{b}_1^s = \mathbf{b}_D = \mathbf{b}_1$. For $\mathbf{b}_2^s$ the vectors $\mathbf{a}_D = -\mathbf{b}_3$, $\mathbf{c}_D = \mathbf{b}_2 - \mathbf{b}_1$, $\mathbf{d}_D = \mathbf{b}_3 - \mathbf{b}_1$ and $(\mathbf{b}_D + \mathbf{c}_D) = \mathbf{b}_2$ are possible. $\mathbf{b}_3^s$ can only be chosen from these vectors such that a linear independent triplet results.

The resulting five choices are given in Table 3.1.2.5. Any case corresponds to eight combinations of signs for the three basis vectors. The principle of the 'homogenous corner' (*i.e.*, there is always a pair of opposite corners of the corresponding cell where all angles are either non-acute or all three are acute) selects one of the bases in each case, thus five different bases remain. For the final choice the surfaces of the corresponding cells are given.

The maximal surface has cell No. 1 with the metrical parameters

$a = 2.449, b = c = 2.828$ Å, $\alpha = 104.47, \beta = 115.66, \gamma = 106.78°$.

A last possibility for the standardization is the interchange of **b** and **c** with inversion of all basis vectors. In this way the sequence of β and γ can be interchanged:

$a = 2.449, b = c = 2.828$ Å, $\alpha = 104.47, \beta = 106.78, \gamma = 115.66°$.

Table 3.1.2.4
Delaunay reduction for Gruber's example

a	**b**	**c**	**d**	**ab**, $\mathbf{a}_D\mathbf{b}_D$	**ac**, $\mathbf{a}_D\mathbf{c}_D$	**ad**, $\mathbf{a}_D\mathbf{d}_D$	**bc**, $\mathbf{b}_D\mathbf{c}_D$	**bd**, $\mathbf{b}_D\mathbf{d}_D$	**cd**, $\mathbf{c}_D\mathbf{d}_D$	$\mathbf{a}_D$	$\mathbf{b}_D$	$\mathbf{c}_D$	$\mathbf{d}_D$
$\mathbf{b}_2$	$\mathbf{b}_3$	$\mathbf{b}_1$	$\mathbf{b}_4$	+4 −4	+3 +7	−15 −11	+2 −10	14 +6	−11 −15	$\mathbf{b}_2$	$-\mathbf{b}_3$	$\mathbf{b}_1 + \mathbf{b}_3$	$\mathbf{b}_4 + \mathbf{b}_3$
$\mathbf{b}_1 + \mathbf{b}_3$	$\mathbf{b}_2$	$-\mathbf{b}_3$	$\mathbf{b}_3 + \mathbf{b}_4$	+7 −7	−10 −3	−15 −8	−4 −4	−11 +3	+6 −1	$\mathbf{b}_1 + \mathbf{b}_3$	$-\mathbf{b}_2$	$\mathbf{b}_2 - \mathbf{b}_3$	$\mathbf{b}_2 + \mathbf{b}_3 + \mathbf{b}_4$
$-\mathbf{b}_1$	$-\mathbf{b}_2$	$\mathbf{b}_2 - \mathbf{b}_3$	$\mathbf{b}_1 + \mathbf{b}_3$	+3 −3	−1 +2	−8 −5	−4 −4	−7 −1	−3 −6	$-\mathbf{b}_1$	$\mathbf{b}_2$	$-\mathbf{b}_3$	$\mathbf{b}_1 - \mathbf{b}_2 + \mathbf{b}_3$
$-\mathbf{b}_3$	$-\mathbf{b}_1$	$\mathbf{b}_2$	$\mathbf{b}_1 - \mathbf{b}_2 + \mathbf{b}_3$	+2 −2	−4 −2	−6 −4	−3 −3	−5 −1	−1 −3	$-\mathbf{b}_3$	$\mathbf{b}_1$	$\mathbf{b}_2 - \mathbf{b}_1$	$\mathbf{b}_3 - \mathbf{b}_1$

3.1.3. Reduced bases

BY P. M. DE WOLFF

3.1.3.1. Introduction

Unit cells are usually chosen according to the conventions mentioned in Section 3.1.1, so one might think that there is no need for another standard choice. This is not true, however; conventions based on symmetry do not always permit unambiguous choice of the unit cell, and unconventional descriptions of a lattice do occur. They are often chosen for good reasons or they may arise from experimental limitations such as may occur, for example, in high-pressure work. So there is a need for normalized descriptions of crystal lattices.

Accordingly, the *reduced basis*[1] (Eisenstein, 1851; Niggli, 1928), which is a primitive basis unique (apart from orientation) for any given lattice, is at present widely used as a means of classifying and identifying crystalline materials. A comprehensive survey of the principles, the techniques and the scope of such applications is given by Mighell (1976). The present contribution merely aims at an exposition of the basic concepts and a brief account of some applications.

The main criterion for the reduced basis is a metric one: choice of the shortest three non-coplanar lattice vectors as basis vectors. Therefore, the resulting bases are, in general, widely different from any symmetry-controlled basis, *cf.* Section 3.1.1.

3.1.3.2. Definition

A primitive basis **a**, **b**, **c** is called a 'reduced basis' if it is right-handed and if the components of the metric tensor $\boldsymbol{G}$ (*cf.* Section 3.1.1)

$$\begin{matrix} \mathbf{a}\cdot\mathbf{a} & \mathbf{b}\cdot\mathbf{b} & \mathbf{c}\cdot\mathbf{c} \\ \mathbf{b}\cdot\mathbf{c} & \mathbf{c}\cdot\mathbf{a} & \mathbf{a}\cdot\mathbf{b} \end{matrix} \qquad (3.1.3.1)$$

satisfy the conditions shown below. The matrix (3.1.3.1) for the reduced basis is called the *reduced form*.

Because of lattice symmetry there can be two or more possible orientations of the reduced basis in a given lattice but, apart from orientation, the reduced basis is unique.

Any basis, reduced or not, determines a unit cell – that is, the parallelepiped of which the basis vectors are edges. In order to test whether a given basis is the reduced one, it is convenient first to find the 'type' of the corresponding unit cell. The type of a cell depends on the sign of

$$T = (\mathbf{a}\cdot\mathbf{b})(\mathbf{b}\cdot\mathbf{c})(\mathbf{c}\cdot\mathbf{a}).$$

If $T > 0$, the cell is of type I, if $T \leq 0$ it is of type II. 'Type' is a property of the cell since T keeps its value when **a**, **b** or **c** is inverted. Geometrically speaking, such an inversion corresponds to moving the origin of the basis towards another corner of the cell. Corners with all three angles acute occur for cells of type I (one opposite pair, the remaining six corners having one acute and two obtuse angles). The other alternative, specified by main condition (ii) of Section 3.1.3.3, *viz* all three angles non-acute, occurs for cells of type II (one or more opposite pairs, the remaining corners having either one or two acute angles).

The conditions can all be stated analytically in terms of the components (3.1.3.1), as follows:

(*a*) Type-I cell

Main conditions:

$$\mathbf{a}\cdot\mathbf{a} \leq \mathbf{b}\cdot\mathbf{b} \leq \mathbf{c}\cdot\mathbf{c}; \quad |\mathbf{b}\cdot\mathbf{c}| \leq \tfrac{1}{2}\mathbf{b}\cdot\mathbf{b}; \quad |\mathbf{a}\cdot\mathbf{c}| \leq \tfrac{1}{2}\mathbf{a}\cdot\mathbf{a}; \quad |\mathbf{a}\cdot\mathbf{b}| \leq \tfrac{1}{2}\mathbf{a}\cdot\mathbf{a} \qquad (3.1.3.2a)$$

$$\mathbf{b}\cdot\mathbf{c} > 0; \quad \mathbf{a}\cdot\mathbf{c} > 0; \quad \mathbf{a}\cdot\mathbf{b} > 0. \qquad (3.1.3.2b)$$

Special conditions:

$$\text{if } \mathbf{a}\cdot\mathbf{a} = \mathbf{b}\cdot\mathbf{b} \text{ then } \mathbf{b}\cdot\mathbf{c} \leq \mathbf{a}\cdot\mathbf{c} \qquad (3.1.3.3a)$$

$$\text{if } \mathbf{b}\cdot\mathbf{b} = \mathbf{c}\cdot\mathbf{c} \text{ then } \mathbf{a}\cdot\mathbf{c} \leq \mathbf{a}\cdot\mathbf{b} \qquad (3.1.3.3b)$$

$$\text{if } \mathbf{b}\cdot\mathbf{c} = \tfrac{1}{2}\mathbf{b}\cdot\mathbf{b} \text{ then } \mathbf{a}\cdot\mathbf{b} \leq 2\mathbf{a}\cdot\mathbf{c} \qquad (3.1.3.3c)$$

$$\text{if } \mathbf{a}\cdot\mathbf{c} = \tfrac{1}{2}\mathbf{a}\cdot\mathbf{a} \text{ then } \mathbf{a}\cdot\mathbf{b} \leq 2\mathbf{b}\cdot\mathbf{c} \qquad (3.1.3.3d)$$

$$\text{if } \mathbf{a}\cdot\mathbf{b} = \tfrac{1}{2}\mathbf{a}\cdot\mathbf{a} \text{ then } \mathbf{a}\cdot\mathbf{c} \leq 2\mathbf{b}\cdot\mathbf{c}. \qquad (3.1.3.3e)$$

(*b*) Type-II cell

Main conditions:

$$\text{as (3.1.3.2}a\text{)} \qquad (3.1.3.4a)$$

$$(|\mathbf{b}\cdot\mathbf{c}| + |\mathbf{a}\cdot\mathbf{c}| + |\mathbf{a}\cdot\mathbf{b}|) \leq \tfrac{1}{2}(\mathbf{a}\cdot\mathbf{a} + \mathbf{b}\cdot\mathbf{b}) \qquad (3.1.3.4b)$$

$$\mathbf{b}\cdot\mathbf{c} \leq 0; \quad \mathbf{a}\cdot\mathbf{c} \leq 0; \quad \mathbf{a}\cdot\mathbf{b} \leq 0. \qquad (3.1.3.4c)$$

Special conditions:

$$\text{if } \mathbf{a}\cdot\mathbf{a} = \mathbf{b}\cdot\mathbf{b} \text{ then } |\mathbf{b}\cdot\mathbf{c}| \leq |\mathbf{a}\cdot\mathbf{c}| \qquad (3.1.3.5a)$$

$$\text{if } \mathbf{b}\cdot\mathbf{b} = \mathbf{c}\cdot\mathbf{c} \text{ then } |\mathbf{a}\cdot\mathbf{c}| \leq |\mathbf{a}\cdot\mathbf{b}| \qquad (3.1.3.5b)$$

$$\text{if } |\mathbf{b}\cdot\mathbf{c}| = \tfrac{1}{2}\mathbf{b}\cdot\mathbf{b} \text{ then } \mathbf{a}\cdot\mathbf{b} = 0 \qquad (3.1.3.5c)$$

$$\text{if } |\mathbf{a}\cdot\mathbf{c}| = \tfrac{1}{2}\mathbf{a}\cdot\mathbf{a} \text{ then } \mathbf{a}\cdot\mathbf{b} = 0 \qquad (3.1.3.5d)$$

$$\text{if } |\mathbf{a}\cdot\mathbf{b}| = \tfrac{1}{2}\mathbf{a}\cdot\mathbf{a} \text{ then } \mathbf{a}\cdot\mathbf{c} = 0 \qquad (3.1.3.5e)$$

$$\text{if } (|\mathbf{b}\cdot\mathbf{c}| + |\mathbf{a}\cdot\mathbf{c}| + |\mathbf{a}\cdot\mathbf{b}|) = \tfrac{1}{2}(\mathbf{a}\cdot\mathbf{a} + \mathbf{b}\cdot\mathbf{b}) \text{ then } \mathbf{a}\cdot\mathbf{a} \leq 2|\mathbf{a}\cdot\mathbf{c}| + |\mathbf{a}\cdot\mathbf{b}|. \qquad (3.1.3.5f)$$

The geometrical interpretation in the following sections is given in order to make the above conditions more explicit rather than to replace them, since the analytical form is obviously the most suitable one for actual verification.

3.1.3.3. Main conditions

The main conditions[2] express the following two requirements:

(i) Of all lattice vectors, none is shorter than **a**; of those not directed along **a**, none is shorter than **b**; of those not lying in the **ab** plane, none is shorter than **c**. This requirement is expressed analytically by (3.1.3.2*a*), and for type-II cells by (3.1.3.4*b*), which for type-I cells is redundant.

(ii) The three angles between basis vectors are either all acute or all non-acute, conditions (3.1.3.2*b*) and (3.1.3.4*c*). As shown in Section 3.1.3.2 for a given unit cell, the origin corner can always be chosen so as to satisfy either the first alternative of this condition (if the cell is of type I) or the second (if the cell is of type II).

[1] Very often, the term 'reduced cell' is used to indicate this normalized lattice description. To avoid confusion, we shall use 'reduced basis', since it is actually a basis and some of the criteria are related precisely to the difference between unit cells and vector bases.

[2] In a book on reduced cells and on retrieval of symmetry information from lattice parameters, Gruber (1978) reformulated the main condition (i) as a minimum condition on the sum $s = a + b + c$. He also examined the surface areas of primitive unit cells in a given lattice, which are easily shown to be proportional to the corresponding sums $s^* = a^* + b^* + c^*$ for the reciprocal bases. He finds that if there are two or more non-congruent cells with minimum s ('Buerger cells'), these cells always have different values of s^*. Gruber (1989) proposes a new criterion to replace the conditions (3.1.3.2*a*)–(3.1.3.5*f*), *viz* that, among the cells with the minimum s value, the one with the smallest value of s^* be chosen (which need not be the absolute minimum of s^* since that may occur for cells that are not Buerger cells). The analytic form of this criterion is identical to (3.1.3.2*a*)–(3.1.3.5*e*); only (3.1.3.5*f*) is altered. For further details, see Section 3.1.4.

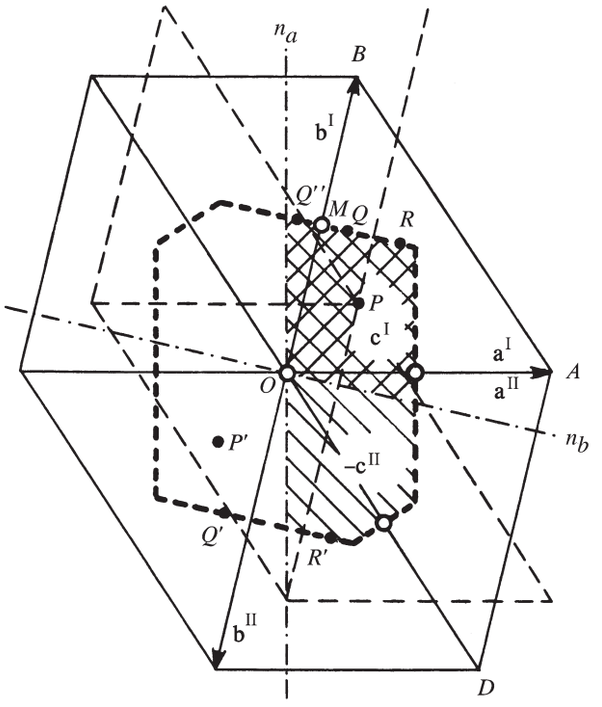


Figure 3.1.3.1
The net of lattice points in the plane of the reduced basis vectors **a** and **b**; *OBAD* is a primitive mesh. The actual choice of **a** and **b** depends on the position of the point *P*, which is the projection of the point P_0 in the next layer (supposed to lie above the paper, thin dashed lines) closest to *O*. Hence, *P* is confined to the Voronoi domain (dashed hexagon) around *O*. For a given interlayer distance, *P* defines the complete lattice. In that sense, *P* and *P*′ represent identical lattices; so do *Q*, *Q*′ and *Q*″, and also *R* and *R*′. When *P* lies in a region marked $-c^{II}$ (hatched), the reduced type-II basis is formed by $\mathbf{a}^{II}$, $\mathbf{b}^{II}$ and $\mathbf{c} = -\overrightarrow{OP}_0$. Regions marked c^I (cross-hatched) have the reduced type-I basis $\mathbf{a}^I$, $\mathbf{b}^I$ and $\mathbf{c} = +\overrightarrow{OP}_0$. Small circles in *O*, *M etc.* indicate twofold rotation points lying on the region borders (see text).

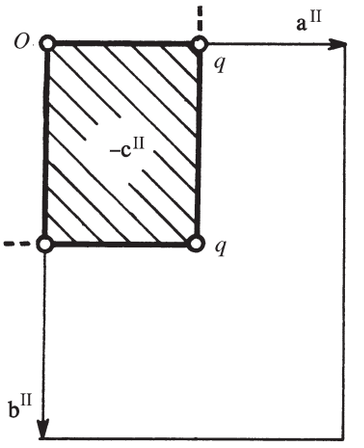


Figure 3.1.3.2
The effect of the special conditions. Border lines of type-I and type-II regions are drawn as heavy lines if included. The type-I and type-II regions are marked as in Fig. 3.1.3.1. A heavy border line of a region stops short of an end point if the latter is not included in the region to which the border belongs. **a**, **b** net primitive orthogonal; special conditions (3.1.3.5*c*), (3.1.3.5*d*).

Condition (i) is by far the most essential one. It uniquely defines the lengths *a*, *b* and *c*, and limits the angles to the range $60 \leq \alpha, \beta, \gamma \leq 120°$. However, there are often different unit cells satisfying (i), *cf.* Gruber (1973). In order to find the reduced basis, starting from an arbitrary one given by its matrix (3.1.3.1), one can: (*a*) find some basis satisfying (i) and (ii) and if necessary modify it so as to fulfil the special conditions as well; (*b*) find all bases satisfying (i) and (ii) and test them one by one with regard to the special conditions until the reduced form is found. Method (*a*) relies mainly on an algorithm by Buerger (1957, 1960), *cf.* also Mighell (1976). Method (*b*) stems from a theorem and an algorithm, both derived by Delaunay (1933); the theorem states that the desired basis vectors **a**, **b** and **c** are among seven (or fewer) vectors – the distance vectors between parallel faces of the Voronoi domain – which follow directly from the algorithm. The method has been established and an example is given by Delaunay *et al.* (1973), *cf.* Section 3.1.2.3 where this method is described.

3.1.3.4. Special conditions

For a given lattice, the main condition (i) defines not only the lengths *a*, *b*, *c* of the reduced basis vectors but also the plane containing **a** and **b**, in the sense that departures from special conditions can be repaired by transformations which do not change this plane. An exception can occur when $b = c$; then such transformations must be supplemented by interchange(s) of **b** and **c** whenever either (3.1.3.3*b*) or (3.1.3.5*b*) is not fulfilled. All the other conditions can be conveniently illustrated by projections of part of the lattice onto the **ab** plane as shown in Figs. 3.1.3.1 to 3.1.3.5. Let us represent the vector lattice by a point lattice. In Fig. 3.1.3.1, the net in the **ab** plane (of which *OBAD* is a primitive mesh; $OA = a$, $OB = b$) is shown as well as the projection (normal to that plane) of the adjoining layer which is assumed to lie above the paper. In general, just one lattice node P_0 of that layer, projected in Fig. 3.1.3.1 as *P*, will be closer to the origin than all others. Then the vector $\overrightarrow{OP}_0$ is $\pm\mathbf{c}$ according to condition (i). It should be stressed that, though the **ab** plane is most often (see above) correctly established by (i), the vectors **a**, **b** and **c** still have to be chosen so as to comply with (ii), with the special conditions, and with right-handedness. The result will depend on the position of *P* with respect to the net. This dependence will now be investigated.

The inner hexagon shown, which is the two-dimensional Voronoi domain around *O*, limits the possible projected positions *P* of P_0. Its short edges, normal to *OD*, result from (3.1.3.4*b*); the other edges from (3.1.3.2*a*). If the spacing *d* between **ab** net planes is smaller than *b*, the region allowed for *P* is moreover limited inwardly by the circle around *O* with radius $(b^2 - d^2)^{1/2}$, corresponding to the projection of points P_0 for which $OP_0 = c = b$. The case $c = b$ has been dealt with, so in order to simplify the drawings we shall assume $d > b$. Then, for a given value of *d*, each point within the above-mentioned hexagonal domain, regarded as the projection of a lattice node P_0 in the next layer, completely defines a lattice based on $\overrightarrow{OA}$, $\overrightarrow{OB}$ and $\overrightarrow{OP}_0$. Diametrically opposite points like *P* and *P*′ represent the same lattice in two orientations differing by a rotation of 180° in the plane of the figure. Therefore, the systematics of reduced bases can be shown completely in just half the domain. As a halving line, the n_a normal to *OA* is chosen. This is an important boundary in view of condition (ii), since it separates points *P* for which the angle between OP_0 and *OA* is acute from those for which it is obtuse.

Similarly, n_b, normal to *OB*, separates the sharp and obtuse values of the angles P_0OB. It follows that if *P* lies in the obtuse sector (cross-hatched area) between n_a and n_b, the reduced cell is

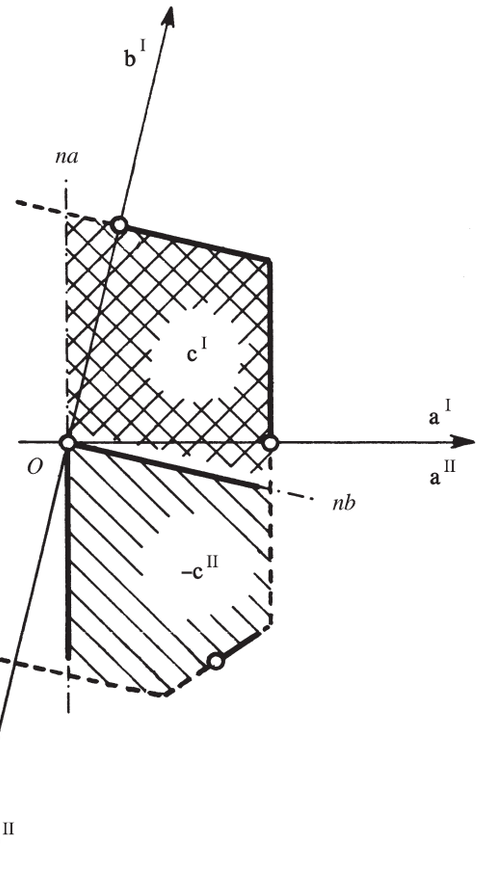


Figure 3.1.3.3
The effect of the special conditions. Border lines of type-I and type-II regions are drawn as heavy lines if included. Type-I and type-II regions are marked as in Fig. 3.1.3.1. n_b belongs to the type-II region. A heavy border line of a region stops short of an end point if the latter is not included in the region to which the border belongs. **a**, **b** net oblique; special conditions (3.1.3.3*c*), (3.1.3.3*d*), (3.1.3.5*f*).

of type I, with basis vectors $\mathbf{a}^{\rm I}$, $\mathbf{b}^{\rm I}$, and $OP_0 = +\mathbf{c}$. Otherwise (hatched area), we have a type-II reduced cell, with $OP_0 = -\mathbf{c}$ and $+\mathbf{a}$ and $+\mathbf{b}$ as shown by $\mathbf{a}^{\rm II}$ and $\mathbf{b}^{\rm II}$.

Since type II includes the case of right angles, the borders of this region on n_a and n_b are inclusive. Other borderline cases are points like R and R', separated by **b** and thus describing the same lattice. By condition (3.1.3.5*c*) the reduced cell for such cases is excluded from type II (except for rectangular **a**, **b** nets, *cf.* Fig. 3.1.3.2); so the projection of **c** points to R, not R'. Accordingly, this part of the border is inclusive for the type-I region and exclusive (at R') for the type-II region as indicated in Fig. 3.1.3.3. Similarly, (3.1.3.5*d*) defines which part of the border normal to OA is inclusive.

The inclusive border is seen to end where it crosses OA, OB or OD. This is prescribed by the conditions (3.1.3.3*d*), (3.1.3.3*c*) and (3.1.3.5*f*), respectively. The explanation is given in Fig. 3.1.3.1 for (3.1.3.3*c*): The points Q and Q'' represent the same lattice because Q' (diametrically equivalent to Q as shown before) is separated from Q'' by the vector **b**. Hence, the point M halfway between O and B is a twofold rotation point just like O. For a primitive orthogonal **a**, **b** net, only type II occurs according to (3.1.3.5*c*) and (3.1.3.5*d*), *cf.* Fig. 3.1.3.2. A centred orthogonal **a**, **b** net of elongated character (shortest net vector in a symmetry direction, *cf.* Section 3.1.3.5) is depicted in Fig. 3.1.3.4. It yields type-I cells except when $\beta = 90°$ [condition (3.1.3.5*c*)]. Moreover, (3.1.3.3*c*) eliminates part of the type-I region as compared to Fig.

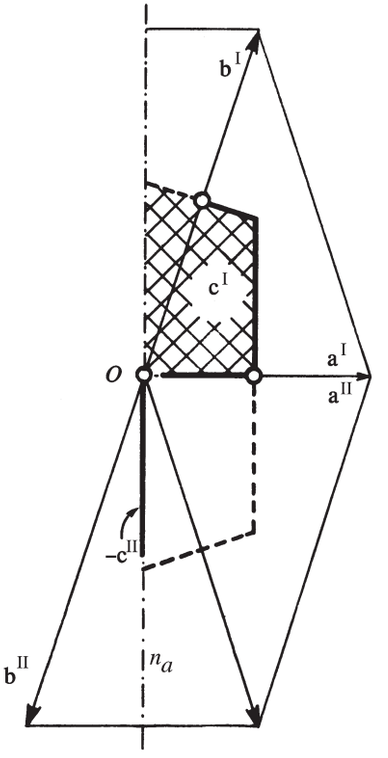


Figure 3.1.3.4
The effect of the special conditions. Border lines of type-I and type-II regions are drawn as heavy lines if included. The type-I region is cross-hatched; the type-II region is a mere line. A heavy border line of a region stops short of an end point if the latter is not included in the region to which the border belongs. **a**, **b** net centred orthogonal (elongated); special conditions (3.1.3.3*e*), (3.1.3.5*e*).

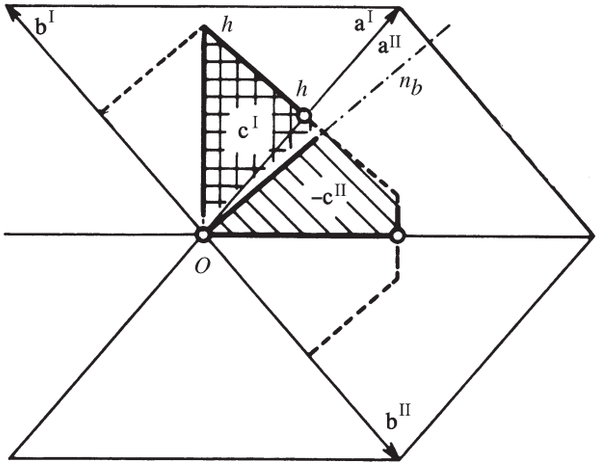


Figure 3.1.3.5
The effect of the special conditions. Border lines of type-I and type-II regions are drawn as heavy lines if included. Type-I and type-II regions are marked as in Fig. 3.1.3.1. n_b belongs to the type-II region. A heavy border line of a region stops short of an end point if the latter is not included in the region to which the border belongs. **a**, **b** net centred orthogonal (compressed); special conditions (3.1.3.3*a*), (3.1.3.5*a*).

3.1.3.3. Finally, a centred net with compressed character (shortest two net vectors equal in length) requires criteria allowing unambiguous designation of **a** and **b**. These are conditions (3.1.3.3*a*) and (3.1.3.5*a*), *cf.* Fig. 3.1.3.5. The simplicity of these bisecting conditions, similar to those for the case $b = c$ mentioned initially, is apparent from that figure when compared

Table 3.1.3.1
The parameters $D = \mathbf{b}\cdot\mathbf{c}$, $E = \mathbf{a}\cdot\mathbf{c}$ and $F = \mathbf{a}\cdot\mathbf{b}$ of the 44 lattice characters ($A = \mathbf{a}\cdot\mathbf{a}$, $B = \mathbf{b}\cdot\mathbf{b}$, $C = \mathbf{c}\cdot\mathbf{c}$)

The character of a lattice given by its reduced form (3.1.3.1) is the first one that agrees when the 44 entries are compared with that reduced form in the sequence given below (suggested by Gruber). Such a logical order is not always obeyed by the widely used character numbers (first column), which therefore show some reversals, *e.g.* 4 and 5.

No.	Type	D	E	F	Lattice symmetry	Bravais type of lattice†	Transformation to a conventional basis (*cf.* footnote ‡ to Table 3.1.3.2)
$A = B = C$							
1	I	$A/2$	$A/2$	$A/2$	Cubic	*cF*	$1\bar{1}1/11\bar{1}/\bar{1}11$
2	I	D	D	D	Rhombohedral	*hR*	$1\bar{1}0/101/\bar{1}\bar{1}\bar{1}$
3	II	0	0	0	Cubic	*cP*	100/010/001
5	II	$-A/3$	$-A/3$	$-A/3$	Cubic	*cI*	101/110/011
4	II	D	D	D	Rhombohedral	*hR*	$1\bar{1}0/\bar{1}01/\bar{1}\bar{1}\bar{1}$
6	II	D‡	D	F	Tetragonal	*tI*	011/101/110
7	II	D‡	E	E	Tetragonal	*tI*	101/110/011
8	II	D‡	E	F	Orthorhombic	*oI*	$\bar{1}\bar{1}0/\bar{1}01/0\bar{1}\bar{1}$
$A = B$, no conditions on C							
9	I	$A/2$	$A/2$	$A/2$	Rhombohedral	*hR*	$100/\bar{1}10/\bar{1}\bar{1}3$
10	I	D	D	F	Monoclinic	*mC*	$110/1\bar{1}0/00\bar{1}$
11	II	0	0	0	Tetragonal	*tP*	100/010/001
12	II	0	0	$-A/2$	Hexagonal	*hP*	100/010/001
13	II	0	0	F	Orthorhombic	*oC*	$110/\bar{1}10/001$
15	II	$-A/2$	$-A/2$	0	Tetragonal	*tI*	$\underline{1}00/0\underline{1}0/112$
16	II	D‡	D	F	Orthorhombic	*oF*	$\bar{1}\bar{1}0/\bar{1}10/112$
14	II	D	D	F	Monoclinic	*mC*	$110/\bar{1}10/001$
17	II	D‡	E	F	Monoclinic	*mC*	$1\bar{1}0/110/\bar{1}01$
$B = C$, no conditions on A							
18	I	$A/4$	$A/2$	$A/2$	Tetragonal	*tI*	$0\bar{1}1/1\bar{1}\bar{1}/100$
19	I	D	$A/2$	$A/2$	Orthorhombic	*oI*	$\bar{1}00/0\bar{1}1/\bar{1}11$
20	I	D	E	E	Monoclinic	*mC*	$011/01\bar{1}/100$
21	II	0	0	0	Tetragonal	*tP*	010/001/100
22	II	$-B/2$	0	0	Hexagonal	*hP*	010/001/100
23	II	D	0	0	Orthorhombic	*oC*	$011/0\bar{1}1/100$
24	II	D‡	$-A/3$	$-A/3$	Rhombohedral	*hR*	$121/0\bar{1}1/100$
25	II	D	E	E	Monoclinic	*mC*	$011/0\bar{1}1/100$
No conditions on A, B, C							
26	I	$A/4$	$A/2$	$A/2$	Orthorhombic	*oF*	$100/\bar{1}20/\bar{1}02$
27	I	D	$A/2$	$A/2$	Monoclinic	*mC*	$\bar{1}20/\bar{1}00/0\bar{1}1$
28	I	D	$A/2$	$2D$	Monoclinic	*mC*	$\bar{1}00/\bar{1}02/010$
29	I	D	$2D$	$A/2$	Monoclinic	*mC*	$100/1\bar{2}0/00\bar{1}$
30	I	$B/2$	E	$2E$	Monoclinic	*mC*	$010/012/\bar{1}00$
31	I	D	E	F	Triclinic	*aP*	100/010/001
32	II	0	0	0	Orthorhombic	*oP*	100/010/001
40	II	$-B/2$	0	0	Orthorhombic	*oC*	$0\bar{1}0/012/\bar{1}00$
35	II	D	0	0	Monoclinic	*mP*	$0\bar{1}0/\bar{1}00/00\bar{1}$
36	II	0	$-A/2$	0	Orthorhombic	*oC*	$100/\bar{1}02/010$
33	II	0	E	0	Monoclinic	*mP*	100/010/001
38	II	0	0	$-A/2$	Orthorhombic	*oC*	$\bar{1}00/120/00\bar{1}$
34	II	0	0	F	Monoclinic	*mP*	$\bar{1}00/00\bar{1}/0\bar{1}0$
42	II	$-B/2$	$-A/2$	0	Orthorhombic	*oI*	$\bar{1}00/0\bar{1}0/112$
41	II	$-B/2$	E	0	Monoclinic	*mC*	$0\bar{1}2/0\bar{1}0/\bar{1}00$
37	II	D	$-A/2$	0	Monoclinic	*mC*	$102/100/010$
39	II	D	0	$-A/2$	Monoclinic	*mC*	$\bar{1}20/\bar{1}00/00\bar{1}$
43	II	D§	E	F	Monoclinic	*mI*	$\bar{1}00/\bar{1}\bar{1}2/0\bar{1}0$
44	II	D	E	F	Triclinic	*aP*	100/010/001

† The symbols for Bravais types of lattices were adopted by the International Union of Crystallography in 1985; *cf.* de Wolff *et al.* (1985). The capital letter of the symbols in this column indicates the centring type of the cell as obtained by the transformation in the last column. For this reason, the standard symbols *mS* and *oS* are not used here. ‡ $2|D + E + F| = A + B$. § $2|D + E + F| = A + B$ plus $|2D + F| = B$.

with Fig. 3.1.3.3. This compressed type of centred orthogonal **a**, **b** net is limited by the case of a hexagonal net (where it merges with the elongated type, Fig. 3.1.3.4) and by the centred quadratic net (where it merges with the primitive orthogonal net, Fig. 3.1.3.2). In the limit of the hexagonal net, the triangle *Ohh* in Figs. 3.1.3.4 and 3.1.3.5 is all that remains, it is of type I except for the point *O*. For the quadratic net, only the type-II region in Fig. 3.1.3.5, then a triangle with all edges inclusive, is left. It corresponds to the triangle *Oqq* in Fig. 3.1.3.2.

3.1.3.5. Lattice characters

Apart from being unique, the reduced cell has the further advantage of allowing a much finer differentiation between types of lattices than is given by the Bravais types. For two-dimensional lattices, this is apparent already in the last section where the centred orthogonal class is subdivided into nets with elongated character and those with compressed character, depending on whether the shortest net vector is, or is not, a symmetry direction.

Table 3.1.3.2
Lattice characters described by relations between conventional cell parameters

Under each of the roman numerals below 'Lattice characters in', *numbers* of characters (*cf.* Table 3.1.3.1, first column) are listed for which the key parameter p lies in the interval defined by the same roman numeral below 'Intervals of p'. For instance, a lattice with character No. 15 under IV has $p = c/a$; so it falls in the interval IV with $2^{1/2} < c/a$ ($< \infty$); No. 33 under II has $p = b$; therefore the interval $a - c$ for II yields the relation $a < b < c$.

Lattice symmetry	Bravais type of lattice†	p = key parameter	Lattice characters in I	II	III	IV	Intervals of p I	II	III	IV		Conventions‡
Tetragonal	*tP*	c/a	21	11	–	–	0	1	∞	–	–	
Tetragonal	*tI*	c/a	18	6	7	15	0	$(2/3)^{1/2}$	1	$2^{1/2}$	∞	
Hexagonal	*hP*	c/a	22	12	–	–	0	1	∞	–	–	
Rhombohedral	*hR*	c/a	24	4	2	9	0	$(3/8)^{1/2}$	$(3/2)^{1/2}$	$6^{1/2}$	∞	Hexagonal axes
Orthorhombic	*oP*	–	32 no relations				–	–	–	–	–	$a < b < c$
Orthorhombic	*oS*											
$b < a\sqrt{3}$		c	23	13	–	–	0	*d*§	∞	–	–	$a < b$
$b > a\sqrt{3}$		c	40	36	38	–	0	*a*	*d*§	∞	–	
Orthorhombic	*oI*	*r*¶	8	19	42	–	0	*a*	*b*	∞	–	$a < b < c$
Orthorhombic	*oF*	b/a	16	26	–	–	1	$3^{1/2}$	∞	–	–	$a < b < c$
Monoclinic	*mP*	b	35	33	34	–	0	*a*	*c*	∞	–	$a < c$††
Monoclinic	*mS*											
Centred net = 1‡‡		b/a	–	–	–	28 or 29						
Centred net = 2		b/a	–	–	–	30						
Centred net = 2, 3		b/a	37 or 41	20	25	–	0	$(1/3)^{1/2}$	1	$3^{1/2}$	∞	*C* centred††
Centred net = 1, 2, 3		b/a	27 or 39	10 or 17	14	–						
Centred net = 3		b/a	43	–	–	–	1	∞	–	–	–	*I* centred††
Triclinic	*aP*	α, β, γ	31	44	–	–	60°	90°	120°	–	–	$a < b < c$
Cubic	*cP*	–		3	no relations		–	–	–	–	–	
	cI	–		5			–	–	–	–	–	
	cF	–		1			–	–	–	–	–	

† The symbols for Bravais types of lattices were adopted by the International Union of Crystallography in 1985; *cf.* de Wolff *et al.* (1985). ‡ These conventions refer to the cells obtained by the transformations of Table 3.1.3.1. They have been chosen for convenience in this table. § $d = \frac{1}{2}(a^2 + b^2)^{1/2}$. ¶ $r = \frac{1}{2}(a^2 + b^2 + c^2)^{1/2}$. †† Setting with unique axis b; $\beta > 90°$; $a < c$ for both *P* and *I* cells, $a < c$ or $a > c$ for *C* cells. ‡‡ This number specifies the centred net among the three orthogonal nets parallel to the twofold axis and passing through (1) the shortest, (2) the second shortest, and (3) the third shortest lattice vector perpendicular to the axis. For example, '2, 3' means that either net (2) or net (3) is the centred one.

It is impossible to perform a continuous deformation – within the centred orthogonal type – of an elongated net into a compressed one, since one has to pass through either a hexagonal or a quadratic net.

In three dimensions, lattices are of the same character if, first, a continuous deformation of one into the other is possible without leaving the Bravais type. Secondly, it is required that all matrix elements of the reduced form (3.1.3.1) change continuously during such a deformation. These criteria lead to 44 different *lattice characters* (Niggli, 1928; Buerger, 1957). Each of them can be recognized easily from the relations between the elements of the reduced form given in Table 3.1.3.1 [adapted from Table 5.1.3.1 in *International Tables for X-ray Crystallography* (1969), which was improved by Mighell & Rodgers (1980)]. The numbers in column 1 of this table are at the same time used as a general notation of the lattice characters themselves. We speak, for example, about the lattice character No. 7 (which is part of the Bravais type *tI*) *etc*.

In Table 3.1.3.2, another description of lattice characters is given by grouping together all characters of a given Bravais type and by indicating for each character the corresponding interval of values of a suitable parameter p, expressed in the usual parameters of a conventional cell. In systems where no generally accepted convention exists, the choice of this cell has been made for convenience in the last column of this table.

The subdistinctions 'centred net = 1, 2 or 3' for the monoclinic centred type are closely related to the description in other conventions. For instance, they correspond to *C*-, *A*- or *I*-centred cells, respectively, if **b** is the unique axis and **a** and **c** are the shortest vectors ($a < c$) perpendicular to **b**; note that in Table 3.1.3.2 only *C* and *I*, not *A*, cells are listed. From the multiple entries in Table 3.1.3.2 for this type, it follows that the description in terms of *b/a* is not exhaustive; the distinctions depend upon rather intricate relations (*cf.* Mighell *et al.*, 1975; Mighell & Rodgers, 1980).

No attempt has been made in Table 3.1.3.2 to specify whether the end points of p intervals are inclusive or not. For practical purposes, they can always be taken to be non-inclusive. Indeed, the end points correspond either to a different Bravais type or to a purely geometric singularity without physical significance. If p is very close to an interval limit of the latter kind, one should be aware of the fact that different measurements of such a lattice may yield different characters, with totally differing aspects of the reduced form.

3.1.3.6. Applications

Classification. The reduced basis can be used to derive the Bravais-lattice type and the conventional cell parameters, starting from an arbitrary description of the lattice. For this purpose, the reduced form is first derived from the given description, *e.g.* by means of the algorithm of Křivý & Gruber (1976). Subsequently it is compared with the reduced forms (Table 3.1.3.1) for the 44 lattice characters and transformed to the appropriate conventional cell. Thus the reduced cell is helpful as an accessory in classifications based on conventional cells.

Alternatively, the parameters of the reduced form itself (either of the direct lattice or of the reciprocal lattice) can be used as a basis for determinative classification.

Comparison of lattices. Two lattices, defined by their reduced cells, can be compared on a rigorous basis to find out whether they are identical lattices or are related by one cell being a subcell of the other (Santoro *et al.*, 1980).

Further properties of lattices are discussed in Section 3.1.4.

P. M. de Wolff wishes to thank Dr B. Gruber (Prague) and Dr A. Santoro (Washington) for reading the manuscript for Section 3.1.3 and for suggesting several improvements as well as pointing out errors, especially in Tables 3.1.3.1 and 3.1.3.2.

3.1.4. Further properties of lattices

By B. Gruber and H. Grimmer

3.1.4.1. Further kinds of reduced cells

In Section 3.1.3.2, 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 (3.1.3.2*a*) to (3.1.3.5*f*) in Section 3.1.3.2] 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[3] – 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;[4]
(ii) the Buerger cell with maximum surface;
(iii) the Buerger cell with minimum deviation;[5]
(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

$$\text{(i), (ii), (iii), (iv).} \qquad (3.1.4.1)$$

[3] See, however, later parts of this section.
[4] Meaning that this cell has the smallest surface of all Buerger cells of the lattice.
[5] The deviation of a cell is the number $|90^\circ - \alpha| + |90^\circ - \beta| + |90^\circ - \gamma|$.

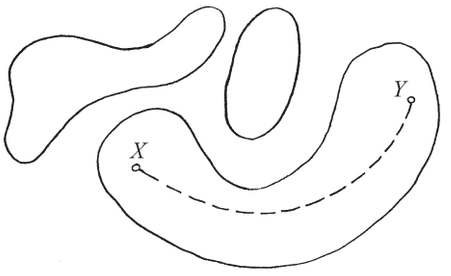


Figure 3.1.4.1
A set **M** in $\mathbb{E}^2$ consisting of three components.

For example, if a lattice has only one Buerger cell, then this cell agrees with all the definitions in (3.1.4.1). However, there exist also Buerger cells that are in agreement with none of them. Thus, the definitions (3.1.4.1) 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 (3.1.4.1) to the reciprocal lattice. Then, to a Buerger cell in the reciprocal lattice, there corresponds a primitive cell with absolute minimum surface[6] in the direct lattice.

The reduced cells according to the definitions (3.1.4.1) 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.

3.1.4.2. Topological characterization 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 **M** of points of the n-dimensional Euclidean space $\mathbb{E}^n$ into equivalence classes called *components* of the set **M**. They can be defined as follows: Two points X, Y of the set **M** belong to the same component if they can be connected by a *continuous* path which lies entirely in the set **M** (Fig. 3.1.4.1). This partition of the set **M** into components is unique and is determined solely by the set **M**.

Now let us return to lattices. To any lattice **L** there is attached a point in $\mathbb{E}^5$ called the *Niggli point* of **L**. It is the point

$$\left[\frac{\mathbf{a}\cdot\mathbf{a}}{\mathbf{c}\cdot\mathbf{c}}, \frac{\mathbf{b}\cdot\mathbf{b}}{\mathbf{c}\cdot\mathbf{c}}, \frac{2\mathbf{b}\cdot\mathbf{c}}{\mathbf{c}\cdot\mathbf{c}}, \frac{2\mathbf{a}\cdot\mathbf{c}}{\mathbf{c}\cdot\mathbf{c}}, \frac{2\mathbf{a}\cdot\mathbf{b}}{\mathbf{c}\cdot\mathbf{c}}\right] \qquad (3.1.4.2)$$

provided that the vectors **a**, **b**, **c** describe the Niggli cell of **L** and fulfil the conditions (3.1.3.2*a*) to (3.1.3.5*f*) of Section 3.1.3.2. 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 $\mathbb{E}^5$ 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 3.1.3.5. 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

[6] This cell need not be a Buerger cell.

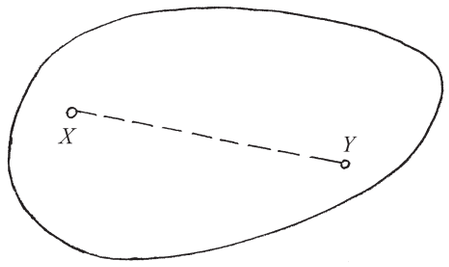


Figure 3.1.4.2
A convex set in $\mathbb{E}^2$.

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. 3.1.4.2). 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:

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 about 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 3.1.3.1 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 (3.1.3.2*a*) to (3.1.3.5*f*) in Section 3.1.3.2 (de Wolff & Gruber, 1991). See also Figs. 3.1.3.1 to 3.1.3.5.

3.1.4.3. 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 3.1.2.3). However, the two 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 by 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.

3.1.4.4. Conventional cells

Conventional cells are dealt with in Section 3.1.1. They are illustrated in Fig. 3.1.2.1 and described in Table 3.1.2.2. This description, however, is not exhaustive enough for determining the Bravais type. In mathematical terms, the conditions in Table 3.1.2.2 are necessary but not sufficient. For example, the *C*-centred cell with

$$a = 6, \quad b = 8, \quad c = 5, \quad \cos\beta = -7/15, \quad \alpha = \gamma = 90^\circ \tag{3.1.4.3}$$

has the typical shape of a conventional cell of an *mC* lattice. But the lattice generated by the *C*-centred cell (3.1.4.3) 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 3.1.4.1. 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 3.1.4.1 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 3.1.4.1. Then a lattice **L** is of this Bravais type if and only if there exists a cell (**a**, **b**, **c**) in **L** such that

Table 3.1.4.1
Conventional cells for the three-dimensional Bravais types of lattices and their limiting cases

All remaining lattices are covered by the anorthic (triclinic) Bravais type *aP*.

Bravais type of lattice	Centring mode of the cell (**a**, **b**, **c**)	Conditions	Limiting cases	Conventional basis (**a**′, **b**′, **c**′) for limiting case
cP	*P*	$a = b = c$, $\alpha = \beta = \gamma = 90^\circ$		
cI	*I*	$a = b = c$, $\alpha = \beta = \gamma = 90^\circ$		
cF	*F*	$a = b = c$, $\alpha = \beta = \gamma = 90^\circ$		
tP	*P*	$a = b \neq c$ $\alpha = \beta = \gamma = 90^\circ$	$b = c \rightarrow cP$	**a**, **b**, **c**
tI	*I*	$c/\sqrt{2} \neq a = b \neq c$, $\alpha = \beta = \gamma = 90^\circ$	$c/\sqrt{2} = a \rightarrow cF$ $b = c \rightarrow cI$	**a** + **b**, **b** − **a**, **c** **a**, **b**, **c**
oP	*P*	$a < b < c$,† $\alpha = \beta = \gamma = 90^\circ$	$a = b \rightarrow tP$ $b = c \rightarrow tP$	**a**, **b**, **c** ($c'/a' > 1$) **b**, **c**, **a** ($c'/a' < 1$)
oI	*I*	$a < b < c$, $\alpha = \beta = \gamma = 90^\circ$	$a = b \rightarrow tI$ $b = c \rightarrow tI$	**a**, **b**, **c** ($c'/a' > 1$) **b**, **c**, **a** ($c'/a' < 1$)
oF	*F*	$a < b < c$, $\alpha = \beta = \gamma = 90^\circ$	$a = b \rightarrow tI$ $b = c \rightarrow tI$	(**a** + **b**)/2, (**b** − **a**)/2, **c** ($c'/a' > 1$) (**b** + **c**)/2, (**c** − **b**)/2, **a** ($c'/a' < 1$)
oC	*C*	$a < b \neq a\sqrt{3}$, $\alpha = \beta = \gamma = 90^\circ$	$a = b \rightarrow tP$ $b = a\sqrt{3} \rightarrow hP$	(**a** + **b**)/2, (**b** − **a**)/2, **c** **a**, (**b** − **a**)/2, **c**
hP	*P*	$a = b$ $\alpha = \beta = 90^\circ$, $\gamma = 120^\circ$		
hR	*P*	$a = b = c$, $\alpha = \beta = \gamma$ $\alpha \neq 60^\circ, \alpha \neq 90^\circ, \alpha \neq \omega$‡	$\alpha = 60^\circ \rightarrow cF$ $\alpha = 90^\circ \rightarrow cP$ $\alpha = \omega \rightarrow cI$	−**a** + **b** + **c**, **a** − **b** + **c**, **a** + **b** − **c** **a**, **b**, **c** **b** + **c**, **c** + **a**, **a** + **b**
mP	*P*	$-2c \cos\beta < a < c$,§ $\alpha = \gamma = 90^\circ < \beta$	$\beta = 90^\circ \rightarrow oP$ $-2c \cos\beta = a \rightarrow oC$ $a = c \rightarrow oC$	−**b**, **a**, **c** if $a > b$ **a**, **b**, **c** if $a < b < c$ **a**, **c**, −**b** if $b > c$ **a**, −2**c** − **a**, **b** ($a'\sqrt{3} < b'$) **a** + **c**, **a** − **c**, **b** ($a'\sqrt{3} > b'$)
mI	*I*	$-c \cos\beta < a < c$,¶ $\alpha = \gamma = 90^\circ < \beta$	$\beta = 90^\circ \rightarrow oI$ $-c \cos\beta = a \rightarrow oC$ $a = c \rightarrow oF$	−**b**, **a**, **c** if $a > b$ **a**, **b**, **c** if $a < b < c$ **a**, **c**, −**b** if $b > c$ **b**, **c** + **a**, **a** if $b < \lvert\mathbf{c} + \mathbf{a}\rvert$ **c** + **a**, −**b**, **a** if $b > \lvert\mathbf{c} + \mathbf{a}\rvert$ **b**, **a** + **c**, **a** − **c** if $\lvert\mathbf{a} + \mathbf{c}\rvert > b$ **a** + **c**, **b**, **c** − **a** if $\lvert\mathbf{a} + \mathbf{c}\rvert < b < \lvert\mathbf{a} - \mathbf{c}\rvert$ **a** + **c**, **a** − **c**, **b** if $b > \lvert\mathbf{a} - \mathbf{c}\rvert$
		but not††	$a^2 + b^2 = c^2$, $a^2 + ac \cos\beta = b^2 \rightarrow hR$	**a**, (**a** − **b** − **c**)/2, (**a** + **b** − **c**)/2 ($\alpha' < 60^\circ$)
		nor	$a^2 + b^2 = c^2$, $b^2 + ac \cos\beta = a^2 \rightarrow hR$	**a**, (**a** + **b** + **c**)/2, (**a** − **b** + **c**)/2 ($60^\circ < \alpha' < 90^\circ$)
		nor nor	$c^2 + 3b^2 = 9a^2$, $c = -3a \cos\beta \rightarrow hR$ $a^2 + 3b^2 = 9c^2$, $a = -3c \cos\beta \rightarrow hR$	−**a**, (**a** − **b** + **c**)/2, (**a** + **b** + **c**)/2 ($90^\circ < \alpha' < \omega$)‡ −**c**, (**a** + **b** + **c**)/2, (**a** − **b** + **c**)/2 ($\omega < \alpha'$)‡

† 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 of lattices. ‡ $\omega = \arccos(-1/3) = 109^\circ 28' 16''$. § This means that **a**, **c** are the shortest non-coplanar lattice vectors in their plane. ¶ This means that **a**, **c** are the shortest non-coplanar lattice vectors in their plane on condition that the cell (**a**, **b**, **c**) is body-centred. †† The reason that the limiting cases of *hR* lattices require two additional equalities is that *hR* lattices have only two independent parameters (a, α), whereas *mI* lattices have four (a, b, c, β). A similar situation holds for the transition from anorthic (triclinic) to monoclinic lattices. See Fig. 3.1.4.3.

(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 3.1.4.1.

For most entries the conditions contain one or more signs of type $<$ or $\neq$. If one of these signs is replaced by the equality sign, a Bravais type of higher symmetry is obtained. These limiting cases are listed in column 4. A particular situation occurs for the Bravais type *mI*. The conditions given for this type in the first two lines of column 3 exclude the limiting cases *oI*, *oC* and *oF* but not *hR*. The latter case is excluded if none of the four pairs of equalities listed in column 4 is satisfied.

In the present section a cell of an *oP*, *oI* or *oF* lattice is considered conventional if it satisfies not only the conditions given in column 2 of Table 3.1.2.2 but also $a < b < c$. Similarly, the additional requirement $a < b$ is made for *oC* and the additional requirements $a < c$ and $\beta > 90^\circ$ for *mP* and *mI*. Column 5 gives a conventional basis (**a**′, **b**′, **c**′) for the limiting case expressed in terms of the conventional basis (**a**, **b**, **c**) for the original Bravais type. The basis is chosen such that handedness is conserved, *i.e.* all bases considered in this section may be regarded as right-handed. Lattices of the same type obtained from a given original Bravais type by a different limit condition differ in the shape of their conventional cell. For example, both limit conditions for the

original type *oP* lead to lattices of type *tP* with axial ratios $c'/a' > 1$ and < 1, respectively, as shown in column 5.

The following examples illustrate the meaning of the information on limiting cases given in Table 3.1.4.1.

(1) Consider the original Bravais type *oF*. If a face-centred cell satisfies $\alpha = \beta = \gamma = 90°$ and $a < b = c$, the lattice will be of type *tI* with conventional basis $(\mathbf{a}', \mathbf{b}', \mathbf{c}') = [(\mathbf{b} + \mathbf{c})/2, (\mathbf{c} - \mathbf{b})/2, \mathbf{a}]$ and axial ratio $c'/a' < 1$.

(2) Consider the original Bravais type *mI*. If a body-centred cell satisfies $-c \cos \beta < a < c$, $\alpha = \gamma = 90° < \beta$, $a^2 + b^2 = c^2$ and $a^2 + ac \cos \beta = b^2$, the lattice will be of type *hR* with conventional basis $(\mathbf{a}', \mathbf{b}', \mathbf{c}') = [\mathbf{a}, (\mathbf{a} - \mathbf{b} - \mathbf{c})/2, (\mathbf{a} + \mathbf{b} - \mathbf{c})/2]$ and rhombohedral angle $\alpha' < 60°$.

The limiting cases given in Table 3.1.4.1 are illustrated in Fig. 3.1.4.3.

Figures similar to Fig. 3.1.4.3 were first published by Hosoya (1979) and, independently, by Klemm (1982). The additions made to this section in this present edition are based on Grimmer (2015).

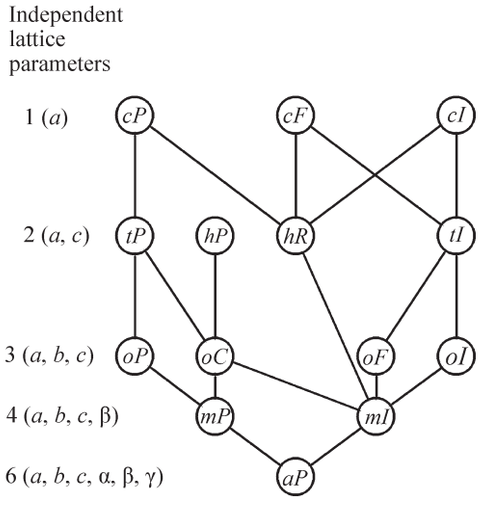


Figure 3.1.4.3
The Bravais-lattice type of the three-dimensional lattice at the upper end of a line is a limiting case of the type at the lower end.

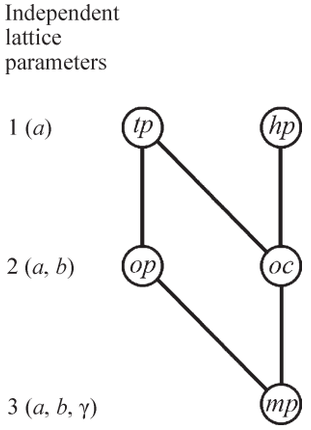


Figure 3.1.4.4
The Bravais-lattice type of the two-dimensional lattice at the upper end of a line is a limiting case of the type at the lower end.

Table 3.1.4.2
Conventional cells for the five two-dimensional Bravais types of lattices and their limiting cases

The centring mode of the cell, *p* or *c*, is indicated in the symbol of the Bravais type.

Bravais type of lattice	Conditions	Limiting cases	Conventional basis $(\mathbf{a}', \mathbf{b}')$ for limiting case
hp	$a = b$, $\gamma = 120°$		
tp	$a = b$, $\gamma = 90°$		
oc	$a < b \neq a\sqrt{3}$, $\gamma = 90°$	$a = b \rightarrow tp$ $a\sqrt{3} = b \rightarrow hp$	$(\mathbf{a} + \mathbf{b})/2, (\mathbf{b} - \mathbf{a})/2$ $\mathbf{a}, (\mathbf{b} - \mathbf{a})/2$
op	$a < b$, $\gamma = 90°$	$a = b \rightarrow tp$	$\mathbf{a}, \mathbf{b}$
mp	$-2b \cos \gamma < a < b$, $90° < \gamma$	$\gamma = 90° \rightarrow op$ $-2b \cos \gamma = a \rightarrow oc$ $a = b \rightarrow oc$	$\mathbf{a}, \mathbf{b}$ $\mathbf{a}, 2\mathbf{b} + \mathbf{a}$ $(a'\sqrt{3} < b')$ $\mathbf{a} + \mathbf{b}, \mathbf{b} - \mathbf{a}$ $(a'\sqrt{3} > b')$

Conventional cells for the five Bravais types of two-dimensional lattices are described and illustrated in Table 3.1.2.1. The conditions given in column 2 of this table are necessary but not always sufficient. Consider the Bravais type whose symbol appears in Table 3.1.4.2 in the *i*th entry of column 1. A two-dimensional lattice **L** is of this Bravais type if and only if there exists a cell $(\mathbf{a}, \mathbf{b})$ with centring mode indicated by the second letter of the Bravais-type symbol and which satisfies the conditions given in the *i*th entry of column 2.

The conditions in the last three entries of column 2 contain one or more signs of type $<$ or $\neq$. If one of these signs is replaced by the equality sign, a Bravais type of higher symmetry is obtained. These limiting cases are listed in column 3 of Table 3.1.4.2. Column 4 gives a conventional basis for the limiting case expressed in terms of the conventional basis for the original Bravais type.

Consider, for example, the original Bravais type *mp*. If a primitive cell satisfies $-2b \cos \gamma = a < b$ and $\gamma > 90°$, the lattice will be of type *oc* with conventional basis $(\mathbf{a}', \mathbf{b}') = (\mathbf{a}, 2\mathbf{b} + \mathbf{a})$ and cell parameters satisfying $a'\sqrt{3} < b'$.

The limiting cases given in Table 3.1.4.2 are illustrated in Fig. 3.1.4.4.

3.1.4.5. Conventional characters

Lattice characters were defined in Section 3.1.4.2 by dividing the Niggli image of a certain Bravais type $\mathscr{T}$ into components. Doing the same – instead of with the Niggli points – with the parameters of conventional cells[7] of lattices of the Bravais type $\mathscr{T}$ we obtain a division of the range[8] 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.

[7] For *aP* lattices, these parameters are derived from the Niggli point [see (3.1.4.2)].
[8] This range is a subset of $\mathbb{E}_k$, where $k \leq 6$.

Table 3.1.4.3
Conventional characters

Bravais type of lattice	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†	$\alpha < 60^\circ$	{9}
	$60^\circ < \alpha < 90^\circ$	{2}
	$90^\circ < \alpha < \omega$‡	{4}
	$\omega < \alpha$	{24}
mP		{33, 34, 35}
mC		{10, 14, 17, 20, 25, 27, 28, 29, 30, 37, 39, 41, 43}
aP	$\alpha < 90^\circ$	{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 $\mathbf{L}'$ of an n-dimensional lattice $\mathbf{L}$ is a proper subset of $\mathbf{L}$ which itself is a lattice of the same dimension as $\mathbf{L}$. A sublattice $\mathbf{L}'$ of $\mathbf{L}$ causes a decomposition of the set $\mathbf{L}$ into, say, i mutually congruent sublattices, $\mathbf{L}'$ itself being one of them (Fig. 3.1.4.5). The number i is called the *index* of the sublattice $\mathbf{L}'$ and indicates how many times $\mathbf{L}'$ is 'diluted' with respect to $\mathbf{L}$.

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 $\mathbf{L}$ 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 $\mathbf{L}$ then primitive bases $\mathbf{a}'_1, \ldots, \mathbf{a}'_n$ of all sublattices of index i of the lattice $\mathbf{L}$ can be found by the relations

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

[9] When choosing their hexagonal description.

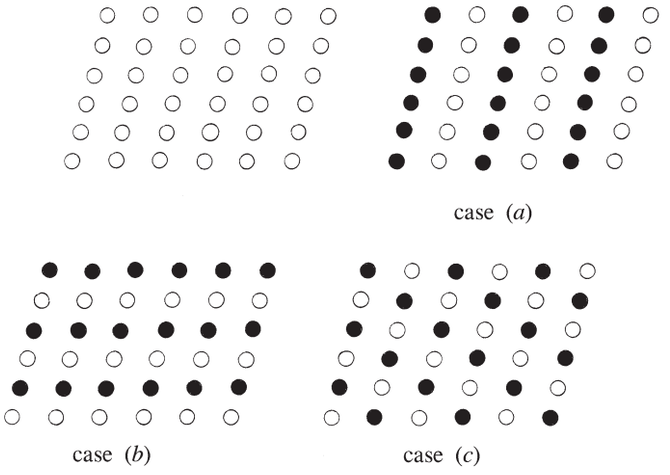


Figure 3.1.4.5
Three possible decompositions of a two-dimensional lattice $\mathbf{L}$ into sublattices of index 2.

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

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

The number $D_{n,i}$ of these matrices is equal to the number of decompositions of an n-dimensional lattice $\mathbf{L}$ 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, 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 $\mathbf{L}$ was irrelevant. We took $\mathbf{L}$ 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 $\mathbf{L}$ 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 $\mathbf{L}$) 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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