International Tables for Crystallography (2016). Vol. A, Section 3.1.3, pp. 709–714.

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.

Copyright © 2016 International Union of Crystallography

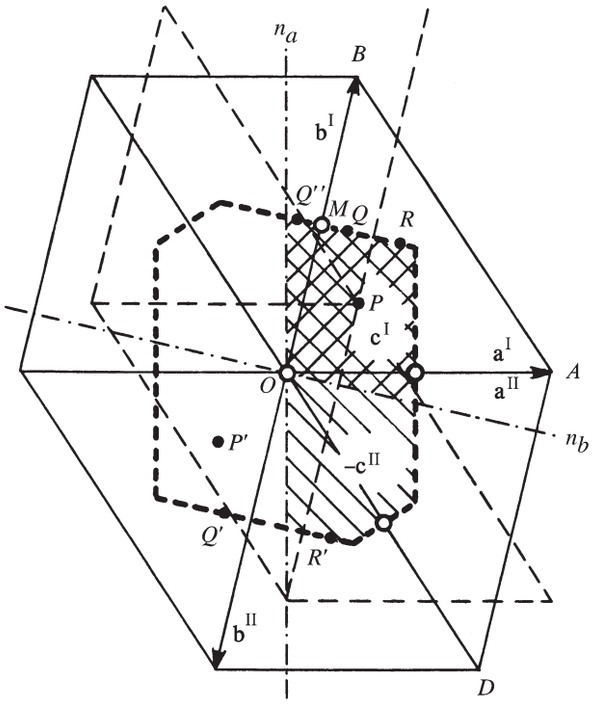

Figure 3.1.3.1
The net of lattice points in the plane of the reduced basis vectors **a** and **b**; *OBAD* is a primitive mesh. The actual choice of **a** and **b** depends on the position of the point *P*, which is the projection of the point P_0 in the next layer (supposed to lie above the paper, thin 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).

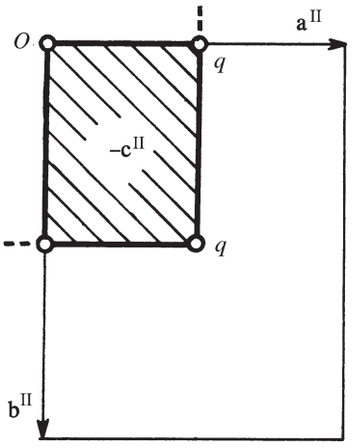

Figure 3.1.3.2
The effect of the special conditions. Border lines of type-I and type-II regions are drawn as heavy lines if included. The type-I and type-II regions are marked as in Fig. 3.1.3.1. A heavy border line of a region stops short of an end point if the latter is not included in the region to 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

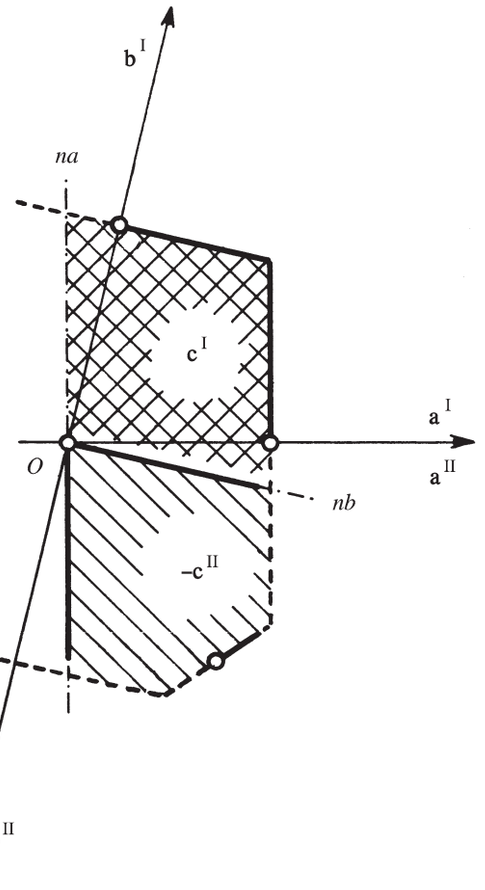

Figure 3.1.3.3
The effect of the special conditions. Border lines of type-I and type-II regions are drawn as heavy lines if included. Type-I and type-II regions are marked as in Fig. 3.1.3.1. n_b belongs to the type-II region. A heavy border line of a region stops short of an end point if the latter 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.

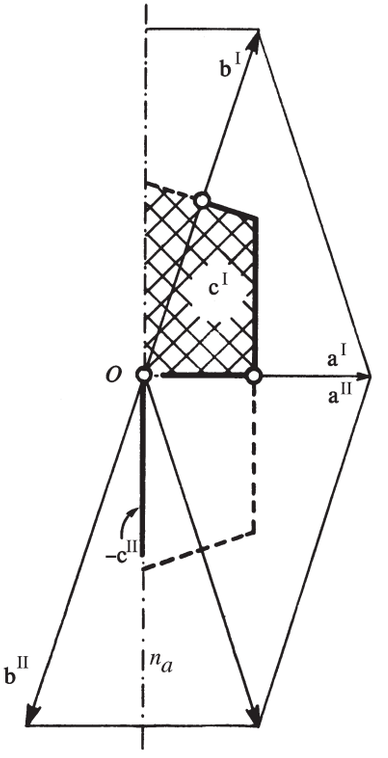

Figure 3.1.3.4
The effect of the special conditions. Border lines of type-I and type-II regions are drawn as heavy lines if included. The type-I region is cross-hatched; the type-II region is a mere line. A heavy border line of a region stops short of an end point if the latter is not included in the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

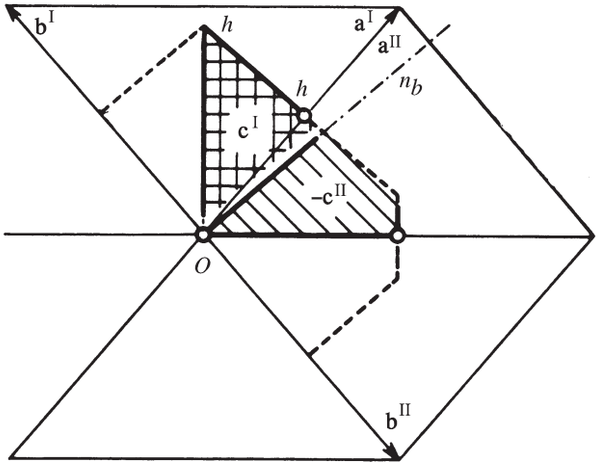

Figure 3.1.3.5
The effect of the special conditions. Border lines of type-I and type-II regions are drawn as heavy lines if included. Type-I and type-II regions are marked as in Fig. 3.1.3.1. n_b belongs to the type-II region. A heavy border line of a region stops short of an end point if the latter 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 $|90^\circ - \alpha| + |90^\circ - \beta| + |90^\circ - \gamma|$.

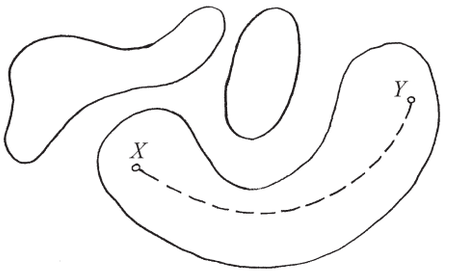

Figure 3.1.4.1
A set **M** in $\mathbb{E}^2$ consisting of three components.

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.