International Tables for Crystallography (2016). Vol. A, Section 3.1.3.4, pp. 710–712.

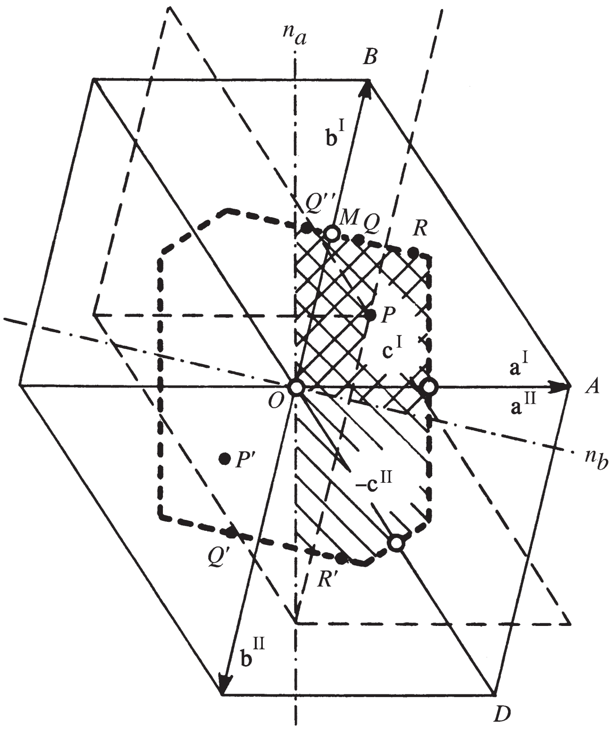

Figure 3.1.3.1
The net of lattice points in the plane of the reduced basis vectors **a** and **b**; *OBAD* is a primitive mesh. The actual choice of **a** and **b** depends on the position of the point *P*, which is the projection of the point P_0 in the next layer (supposed to lie above the paper, thin 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 $-c^{\mathrm{II}}$ (hatched), the reduced type-II basis is formed by $\mathbf{a}^{\mathrm{II}}$, $\mathbf{b}^{\mathrm{II}}$ and $\mathbf{c} = -\overrightarrow{OP}_0$. Regions marked c^{I} (cross-hatched) have the reduced type-I basis $\mathbf{a}^{\mathrm{I}}$, $\mathbf{b}^{\mathrm{I}}$ and $\mathbf{c} = +\overrightarrow{OP}_0$. Small circles in *O*, *M etc.* indicate twofold rotation points lying on the region borders (see text).

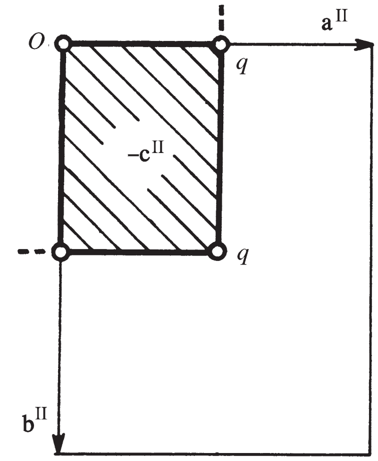

Figure 3.1.3.2
The effect of the special conditions. Border lines of type-I and type-II regions are drawn as heavy lines if included. The type-I and type-II regions are marked as in Fig. 3.1.3.1. A heavy border line of a region stops short of an end point if the latter is not included in the region to 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 $60 \leq \alpha, \beta, \gamma \leq 120^\circ$. 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

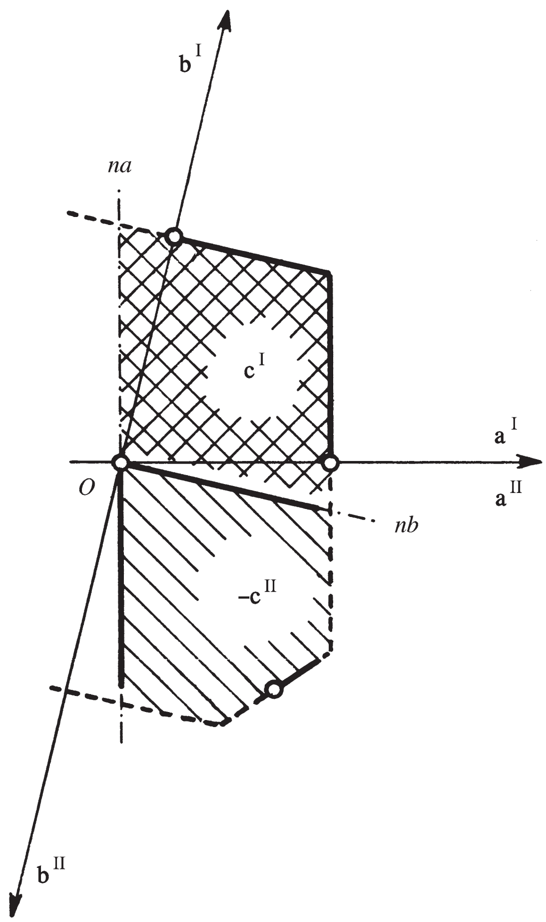

Figure 3.1.3.3
The effect of the special conditions. Border lines of type-I and type-II regions are drawn as heavy lines if included. Type-I and type-II regions are marked as in Fig. 3.1.3.1. n_b belongs to the type-II region. A heavy border line of a region stops short of an end point if the latter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

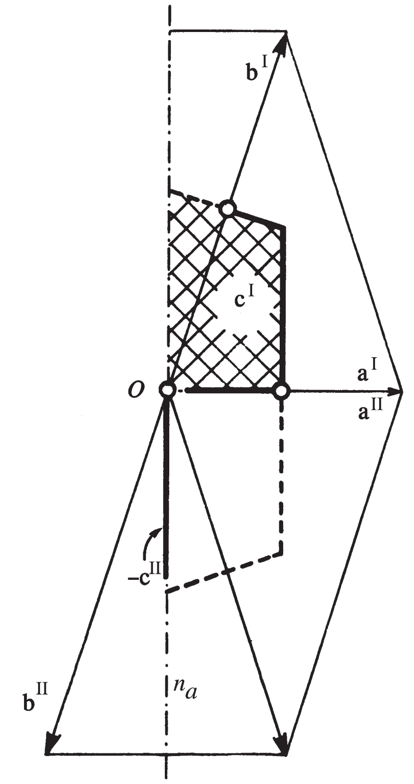

Figure 3.1.3.4
The effect of the special conditions. Border lines of type-I and type-II regions are drawn as heavy lines if included. The type-I region is cross-hatched; the type-II region is a mere line. A heavy border line of a region stops short of an end point if the latter is not included in the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

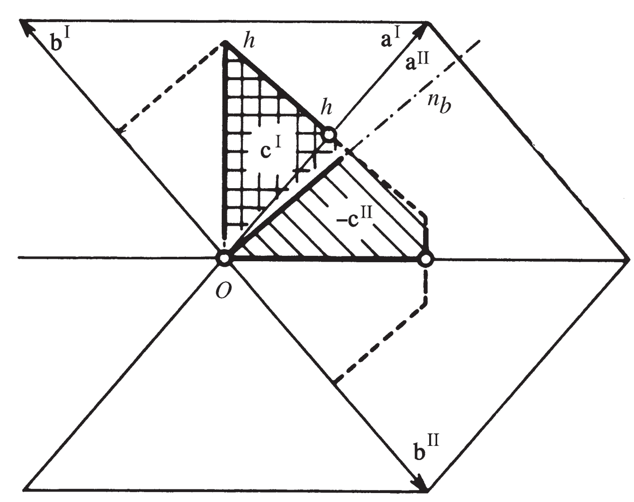

Figure 3.1.3.5
The effect of the special conditions. Border lines of type-I and type-II regions are drawn as heavy lines if included. Type-I and type-II regions are marked as in Fig. 3.1.3.1. n_b belongs to the type-II region. A heavy border line of a region stops short of an end point if the latter 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	$1\bar{1}0/\bar{1}01/\bar{1}\bar{1}\bar{1}$
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	$\bar{1}\bar{1}0/\bar{1}0\bar{1}/0\bar{1}\bar{1}$
$A = B$, 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	100/010/112
16	II	D‡	D	F	Orthorhombic	oF	$\bar{1}\bar{1}0/1\bar{1}0/112$
14	II	D	D	F	Monoclinic	mC	$110/\bar{1}10/001$
17	II	D‡	E	F	Monoclinic	mC	$1\bar{1}0/110/\bar{1}0\bar{1}$
$B = C$, 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	$011/01\bar{1}/\bar{1}00$
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	$010/01\bar{2}/\bar{1}00$
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	$100/\bar{1}0\bar{2}/010$
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	$0\bar{1}\bar{2}/0\bar{1}0/\bar{1}00$
37	II	D	$-A/2$	0	Monoclinic	mC	102/100/010
39	II	D	0	$-A/2$	Monoclinic	mC	$\bar{1}\bar{2}0/\bar{1}00/00\bar{1}$
43	II	D§	E	F	Monoclinic	mI	$\bar{1}00/\bar{1}\bar{1}\bar{2}/0\bar{1}0$
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.

references