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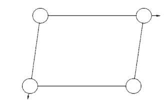
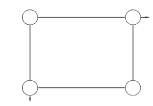
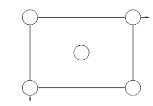
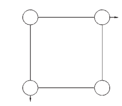
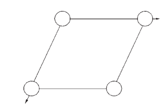
Table 3.1.2.1
Two-dimensional Bravais types of lattices

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

† 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

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

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 $\mathbf{b}_i'^2$ 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.

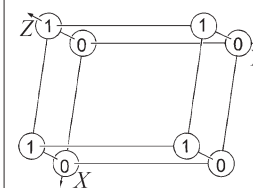
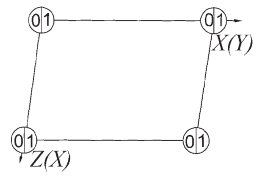
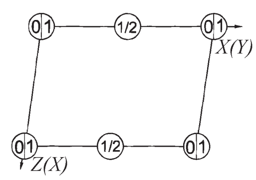
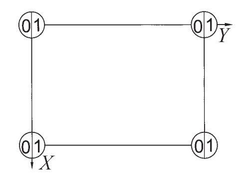
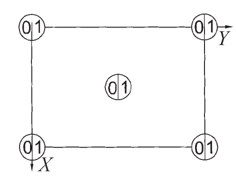
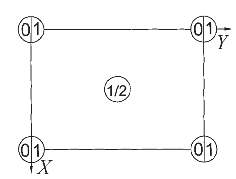
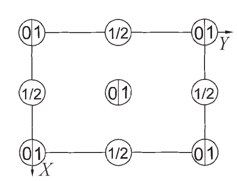
If all the scalar products are less than or equal to zero, the three shortest vectors of the reduced basis are contained in the set $\{\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3, \mathbf{b}_4, \mathbf{b}_1 + \mathbf{b}_2, \mathbf{b}_2 + \mathbf{b}_3, \mathbf{b}_3 + \mathbf{b}_1\}$, called the *Delaunay 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.

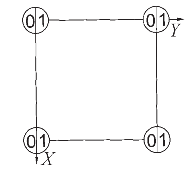
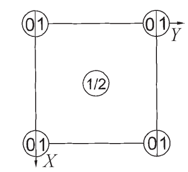
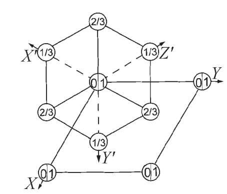
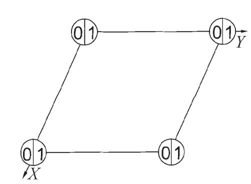
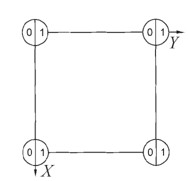
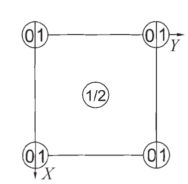
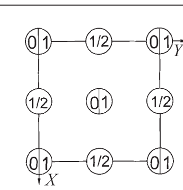
Delaunay combined the topological description with the rotation groups of the crystallographic holohedries. He used upper-case letters for these groups (K – cubic, H – hexagonal, R – rhombohedral, Q – tetragonal, O – orthorhombic, M – monoclinic, T – triclinic) followed by a incremental number if more 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: Conventional	Lattice parameters: Primitive	Metric tensor: Conventional	Metric tensor: Primitive/transf.‡	Metric tensor: Relations of the components	Projections
aP	a, b, c α, β, γ	a, b, c α, β, γ	$\begin{matrix} g_{11} & g_{12} & g_{13} \\ & g_{22} & g_{23} \\ & & g_{33} \end{matrix}$	$\begin{matrix} g_{11} & g_{12} & g_{13} \\ & g_{22} & g_{23} \\ & & g_{33} \end{matrix}$		
mP	a, b, c $\beta, \alpha = \gamma = 90°$	a, b, c $\beta, \alpha = \gamma = 90°$	$\begin{matrix} g_{11} & 0 & g_{13} \\ & g_{22} & 0 \\ & & g_{33} \end{matrix}$	$\begin{matrix} g_{11} & 0 & g_{13} \\ & g_{22} & 0 \\ & & g_{33} \end{matrix}$		
mC (*mS*)		$a_1 = a_2, c$ $\gamma, \alpha = \beta$		$\boldsymbol{P}(C)$ $\begin{matrix} g'_{11} & g'_{12} & g'_{13} \\ & g'_{11} & g'_{13} \\ & & g_{33} \end{matrix}$	$g'_{11} = \frac{1}{4}(g_{11} + g_{22})$ $g'_{12} = \frac{1}{4}(g_{11} - g_{22})$ $g'_{13} = \frac{1}{2}g_{13}$ $g_{11} = 2(g'_{11} + g'_{12})$ $g_{22} = 2(g'_{11} - g'_{12})$ $g_{13} = 2g'_{13}$	
oP	a, b, c $\alpha = \beta = \gamma = 90°$	a, b, c $\alpha = \beta = \gamma = 90°$	$\begin{matrix} g_{11} & 0 & 0 \\ & g_{22} & 0 \\ & & g_{33} \end{matrix}$	$\begin{matrix} g_{11} & 0 & 0 \\ & g_{22} & 0 \\ & & g_{33} \end{matrix}$		
oC (*oS*)		$a_1 = a_2, c$ $\gamma, \alpha = \beta = 90°$		$\boldsymbol{P}(C)$ $\begin{matrix} g'_{11} & g'_{12} & 0 \\ & g'_{11} & 0 \\ & & g_{33} \end{matrix}$	$g'_{11} = \frac{1}{4}(g_{11} + g_{22})$ $g'_{12} = \frac{1}{4}(g_{11} - g_{22})$ $g_{11} = 2(g'_{11} + g'_{12})$ $g_{22} = 2(g'_{11} - g'_{12})$	
oI		$a_1 = a_2 = a_3$ α, β, γ $\cos\alpha + \cos\beta$ $+ \cos\gamma = -1$		$\boldsymbol{P}(I)$ $\begin{matrix} -\tilde{g} & g'_{12} & g'_{13} \\ & -\tilde{g} & g'_{23} \\ & & -\tilde{g} \end{matrix}$ $\tilde{g} = g'_{12} + g'_{13} + g'_{23}$	$g'_{12} = \frac{1}{4}(-g_{11} - g_{22} + g_{33})$ $g'_{13} = \frac{1}{4}(-g_{11} + g_{22} - g_{33})$ $g'_{23} = \frac{1}{4}(g_{11} - g_{22} - g_{33})$ $g_{11} = -2(g'_{12} + g'_{13})$ $g_{22} = -2(g'_{12} + g'_{23})$ $g_{33} = -2(g'_{13} + g'_{23})$	
oF		a, b, c α, β, γ $\cos\alpha = \dfrac{-a^2 + b^2 + c^2}{2bc}$ $\cos\beta = \dfrac{a^2 + b^2 + c^2}{2ac}$ $\cos\gamma = \dfrac{a^2 + b^2 - c^2}{2ab}$		$\boldsymbol{P}(F)$ $\begin{matrix} \tilde{g}_1 & g'_{12} & g'_{13} \\ & \tilde{g}_2 & g'_{23} \\ & & \tilde{g}_3 \end{matrix}$ $\tilde{g}_1 = g'_{12} + g'_{13}$ $\tilde{g}_2 = g'_{12} + g'_{23}$ $\tilde{g}_3 = g'_{13} + g'_{23}$	$g'_{12} = \frac{1}{4}\,g_{33}$ $g'_{13} = \frac{1}{4}\,g_{22}$ $g'_{23} = \frac{1}{4}\,g_{11}$ $g_{11} = 4g'_{23}$ $g_{22} = 4g'_{13}$ $g_{33} = 4g'_{12}$	

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: Conventional	Lattice parameters: Primitive	Metric tensor: Conventional	Metric tensor: Primitive/transf.‡	Metric tensor: Relations of the components	Projections
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. ‡ $\boldsymbol{P}(C) = \frac{1}{2}(110/\bar{1}10/002)$, $\boldsymbol{P}(I) = \frac{1}{2}(\bar{1}11/1\bar{1}1/11\bar{1})$, $\boldsymbol{P}(F) = \frac{1}{2}(011/101/110)$, $\boldsymbol{P}(R) = \frac{1}{3}(\bar{1}2\bar{1}/\bar{2}11/111)$.

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*')

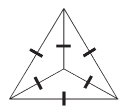
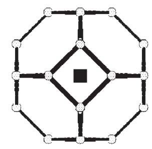
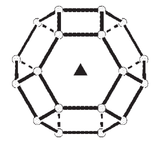
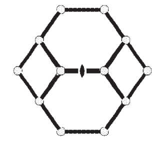
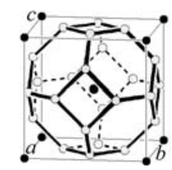
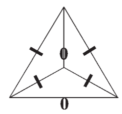
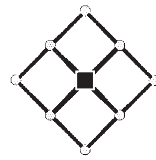
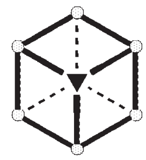
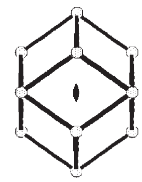
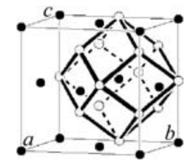
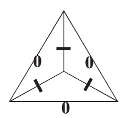
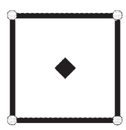
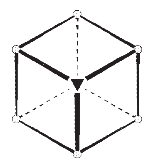
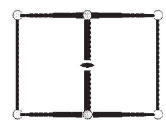
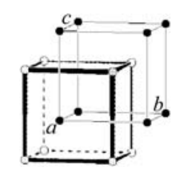
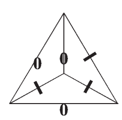
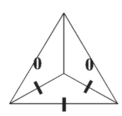
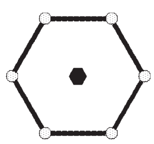
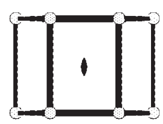
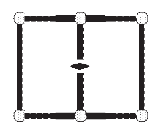
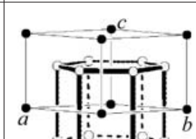
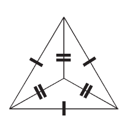
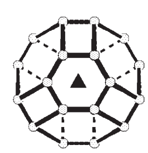
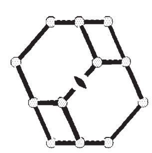
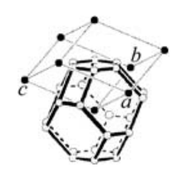
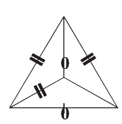
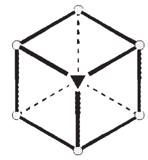
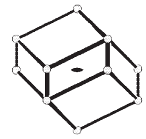
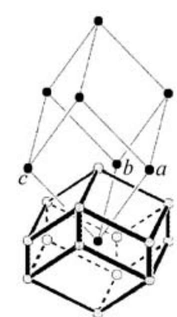
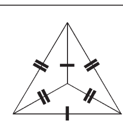
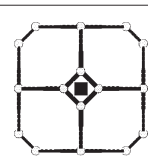
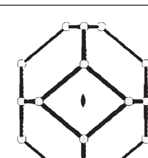
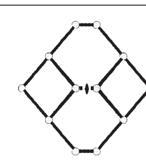
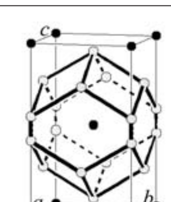
Delaunay–Voronoi type	Metric conditions	Selling tetrahedron	Projections along symmetry directions			Dirichlet domain in the unit cell	Transformation to the conventional cell
*K*1 V1 *cI* $\frac{4}{m}\bar{3}\frac{2}{m}$ $v\ s\ s^2$	—					 	$\begin{pmatrix}0&1&1\\1&0&1\\1&1&0\end{pmatrix}$
*K*2 V3 *cF* $\frac{4}{m}\bar{3}\frac{2}{m}$ $v^4\ v^3\ v$	—					 	$\begin{pmatrix}1&-1&1\\1&1&1\\0&0&2\end{pmatrix}$
*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)

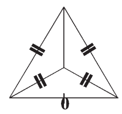
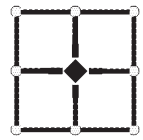
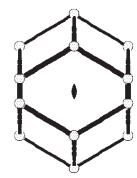
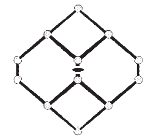
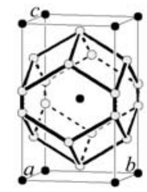
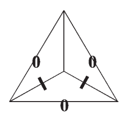
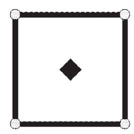
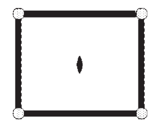
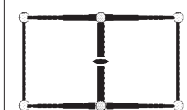
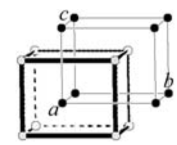
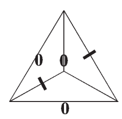
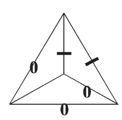
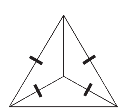
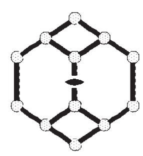
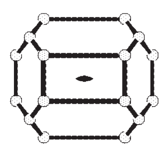
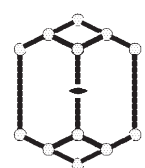
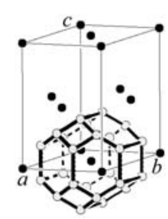
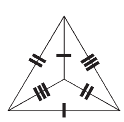
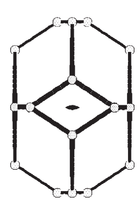
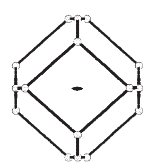
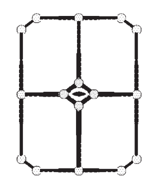
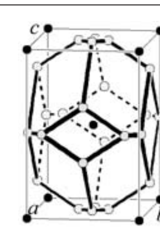
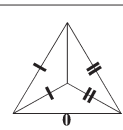
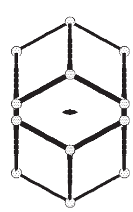
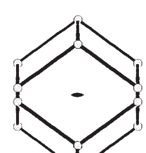
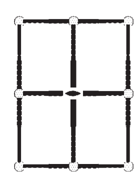
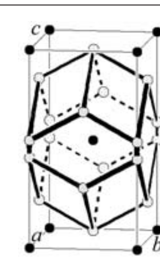
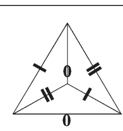
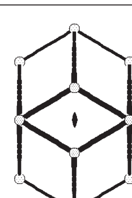
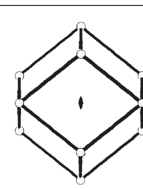
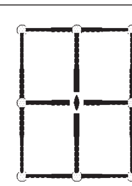
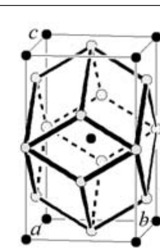
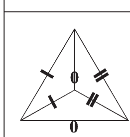
Delaunay–Voronoi type	Metric conditions	Selling tetrahedron	Projections along symmetry directions			Dirichlet domain in the unit cell	Transformation to the conventional cell
*Q*2 V2 *tI* $\frac{4}{m}\frac{2}{m}\frac{2}{m}$ $v^4\ s\ s^2$	$c^2 > 2a^2$						$\begin{pmatrix}1&0&1\\0&1&1\\0&0&2\end{pmatrix}$
*Q*3 V5 *tP* $\frac{4}{m}\frac{2}{m}\frac{2}{m}$ $v\ v\ v^2$	—						$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$
							$\begin{pmatrix}1&0&0\\0&0&1\\0&1&1\end{pmatrix}$
							$\begin{pmatrix}0&0&1\\1&1&0\\0&1&0\end{pmatrix}$
*O*1 V1 *oF* $\frac{2}{m}\frac{2}{m}\frac{2}{m}$ $s^2\ v\ s^2$	—						$\begin{pmatrix}1&-1&1\\1&1&1\\0&0&2\end{pmatrix}$
*O*2 V1 *oI* $\frac{2}{m}\frac{2}{m}\frac{2}{m}$ $v\ v\ v$	$a^2 + b^2 > c^2$						$\begin{pmatrix}0&1&1\\1&0&1\\1&1&0\end{pmatrix}$
*O*3 V2 *oI* $\frac{2}{m}\frac{2}{m}\frac{2}{m}$ $s\ s\ v^4$	$a^2 + b^2 < c^2$						$\begin{pmatrix}1&0&1\\0&1&1\\0&0&2\end{pmatrix}$
*O*4 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)

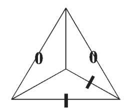
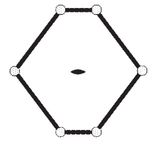
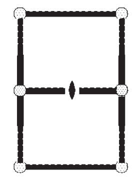
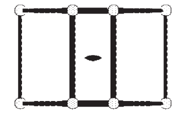
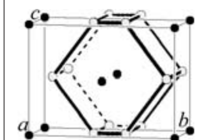
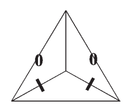
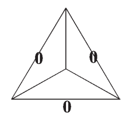
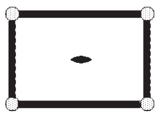
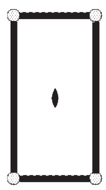
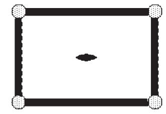
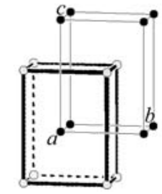
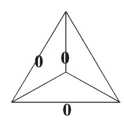
Delaunay–Voronoi type	Metric conditions	Selling tetrahedron	Projections along symmetry directions			Dirichlet domain in the unit cell	Transformation to the conventional cell
*O*5 V4 $o(AB)C$ $\frac{2}{m}\frac{2}{m}\frac{2}{m}$ $s\ v^2\ v$	—						$\begin{pmatrix} 2 & 0 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$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

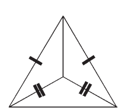
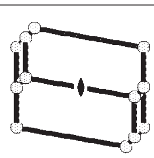
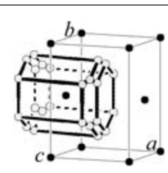
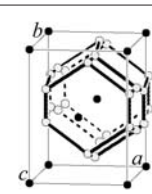
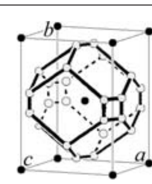
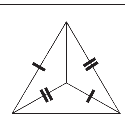
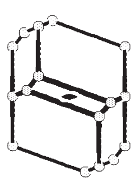
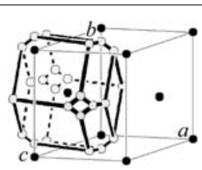
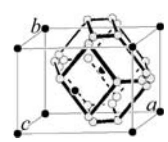
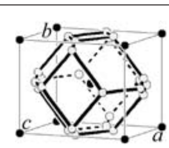
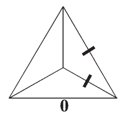
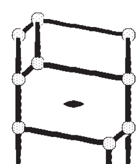
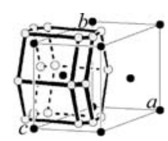
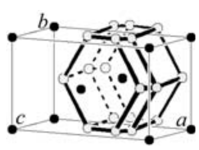
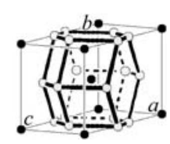
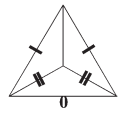
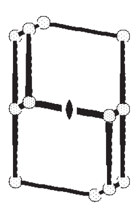
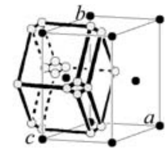
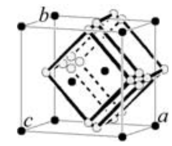
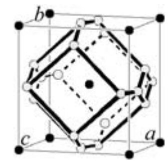
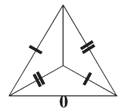
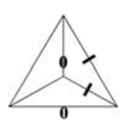
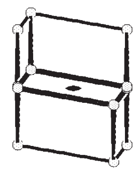
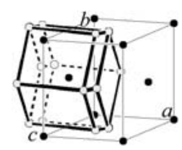
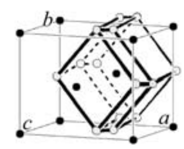
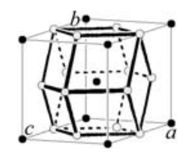
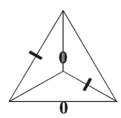
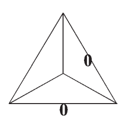
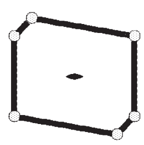
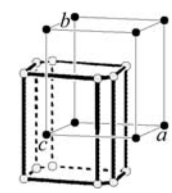
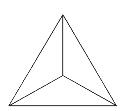
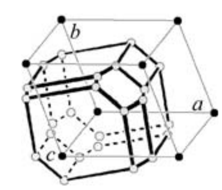
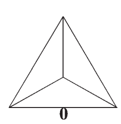
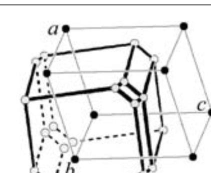
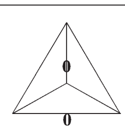
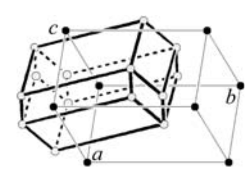
Delaunay–Voronoi type	Metric conditions	Selling tetrahedron	Projections along symmetry directions	Dirichlet domain in the unit cell			Transformation to the conventional cell
*M*1 V1 $m(AC)I$ $\frac{2}{m}$ s^2	$b^2 > p^2$			 *A*: $b^2 > c^2$	 *C*: $b^2 > a^2$	 *I*: $b^2 > f^2$	$\begin{pmatrix} -1 & 1 & 0 \\ -1 & -1 & 0 \\ -1 & 0 & 1 \end{pmatrix}$
*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*	$b^2 = r^2 - q^2$			  	$\begin{pmatrix} -1 & 0 & 1 \\ -1 & 1 & 0 \\ -2 & 0 & 0 \end{pmatrix}$
				*A*: $b^2 = f^2 - a^2$ *C*: $b^2 = f^2 - c^2$ *I*: $b^2 = c^2 - a^2$	$\begin{pmatrix} 1 & 0 & -1 \\ 1 & -1 & 0 \\ 0 & -1 & -1 \end{pmatrix}$
*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), $\beta_{23} = 60^\circ$ ($\cos\beta_{23} = \frac{1}{2}$), $\beta_{13} = 73.22^\circ$ ($\cos\beta_{13} = \sqrt{3}/6$), $\beta_{12} = 64.34^\circ$ ($\cos\beta_{12} = \sqrt{3}/4$).

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

references