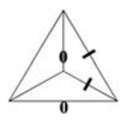
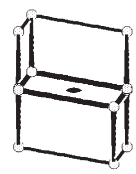
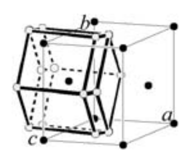
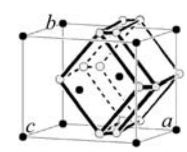
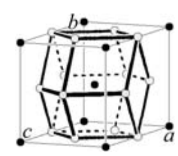
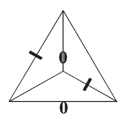
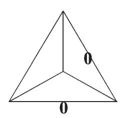
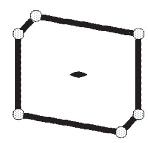
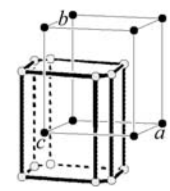
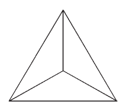
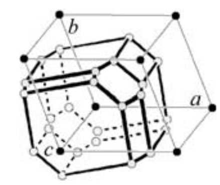
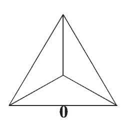
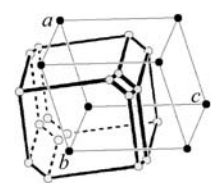
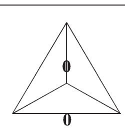
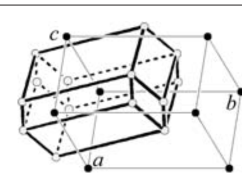
International Tables for Crystallography (2016). Vol. A, Section 3.1.2.4, pp. 707–708.

Table 3.1.2.3 (continued)

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

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

3.1.2.4. Example of Delaunay reduction and standardization of the basis

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

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

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

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

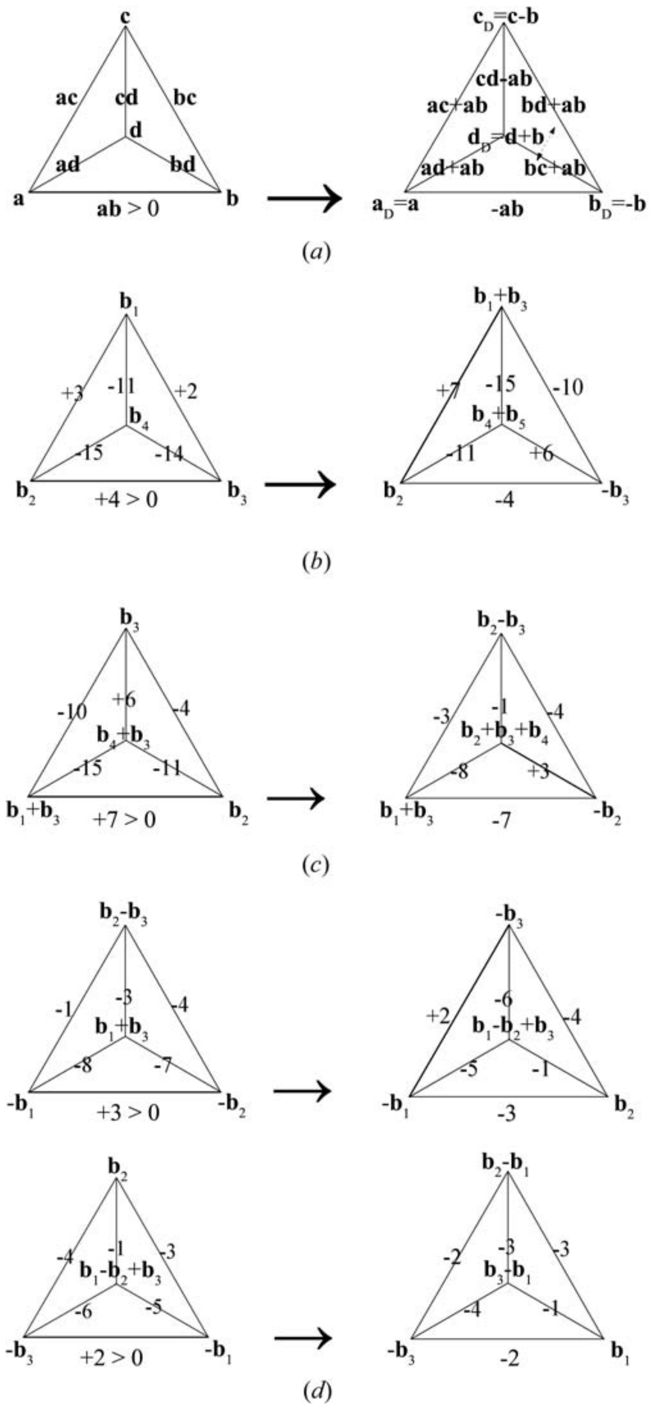


Figure 3.1.2.2
Delaunay reduction of Gruber's example (*cf.* Section 3.1.2.4). The edges of Selling tetrahedra are labelled by the scalar products of the vectors which designate the corners of the tetrahedra.

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

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

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

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

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

For further standardization we consider the Delaunay set

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

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

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

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

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

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

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

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

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

Table 3.1.2.4
Delaunay reduction for Gruber's example

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