International Tables for Crystallography (2006). Vol. A, Section 9.1.9, p. 749.

Table 9.1.9.1. *Example*

Transformation				Scalar products					
				12	13	14	23	24	34
$\mathbf{b}_1$	$\mathbf{b}_2$	$\mathbf{b}_3$	$\mathbf{b}_4$	−0.271	0.265	−22.02	−24.37	0.272	−32.51
$-\mathbf{b}_1$	$\mathbf{b}_1 + \mathbf{b}_2$	$\mathbf{b}_3$	$\mathbf{b}_1 + \mathbf{b}_4$	−21.75	−0.265	0	−24.10	~0	−32.24
$\mathbf{b}_1'$	$\mathbf{b}_3'$	$\mathbf{b}_4'$	$\mathbf{b}_2'$	13	14	12	34	23	24

are considered. The reduction is performed minimizing the sum

$$\textstyle\sum = \mathbf{b}_1{}^2 + \ldots + \mathbf{b}_{n+1}{}^2. \qquad (9.1.8.1)$$

It can be shown that this sum can be reduced 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 performed 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 forming the reduced basis are contained in the set

$$V = \{\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3, \mathbf{b}_4, \mathbf{b}_1 + \mathbf{b}_2, \mathbf{b}_2 + \mathbf{b}_3, \mathbf{b}_3 + \mathbf{b}_1\},$$

which corresponds to the maximal set of faces of the Dirichlet domain (14 faces).

For practical application, it is useful to classify the patterns of the resulting $n(n-1)/2$ scalar products regarding their equivalence or zero values. These classes of patterns correspond to the reduced bases and result in '*Symmetrische Sorten*' (Delaunay, 1933) that lead directly to the conventional crystallographic cells by fixed transformations (*cf.* Patterson & Love, 1957; Burzlaff & Zimmermann, 1993). Table 9.1.8.1 gives the list of the 24 '*symmetrische Sorten*'. Column 1 contains Delaunay's symbols, column 2 the symbol of the Bravais type. For monoclinic centred lattices, the matrix $\boldsymbol{P}$ of the last column transforms the primitive reduced cell into an *I*-centred cell, which has to be transformed to *A* or *C* according to the monoclinic standardization rules, if necessary. $\boldsymbol{P}$ operates on the basis in the following form:

$$(\mathbf{a}_r, \mathbf{b}_r, \mathbf{c}_r) \cdot \boldsymbol{P} = (\mathbf{a}_c, \mathbf{b}_c, \mathbf{c}_c),$$

where $(\mathbf{a}_r, \mathbf{b}_r, \mathbf{c}_r)$ denotes the (1×3) matrix of the basis vectors of the reduced cell and $(\mathbf{a}_c, \mathbf{b}_c, \mathbf{c}_c)$ the (1×3) matrix of the conventional cell.

Column 3 gives metrical conditions for the occurrence of certain Voronoi types. Column 5 indicates the relations among the scalar products of the reduced vector set. 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).

9.1.9. Example

This example is discussed in Azároff & Buerger (1958, pp. 176–180).

The lattice parameters are given as $b_1 = 4.693$, $b_2 = 4.936$, $b_3 = 7.524$ Å, $\beta_{23} = 131.00$, $\beta_{31} = 89.57$, $\beta_{12} = 90.67°$. The scalar products resulting from these data are given in Table 9.1.9.1. The scalar product $\mathbf{b}_1 \cdot \mathbf{b}_3$ is positive. Thus the transformation

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

is applied. The new scalar products are all non-positive as given in the second row of Table 9.1.9.1 (within the accuracy of the experimental data). Comparison with Table 9.1.8.1 leads to *M*6, Voronoi type IV and the monoclinic Bravais lattice *mP*.

The transformation related to this case leads to a monoclinic conventional cell but does not consider the possibility of shorter basis vectors. For this reason, it is necessary here to look at the other vectors of the set *V* in the $(\mathbf{b}_1'\mathbf{b}_3')$ plane, the only one of interest is $\mathbf{b}_1' + \mathbf{b}_3'$. The length of this vector is 4.936 Å, which is shorter than $\mathbf{b}_3'$ ($|\mathbf{b}_3'| = 6.771$ Å) and leads to the cell parameters $a = 4.693, b = 5.678, c = 4.936$ Å, $\alpha = 90, \beta = 90.67, \gamma = 90°$.