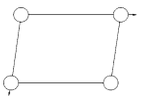
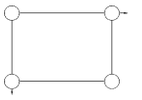
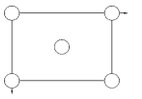
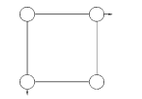
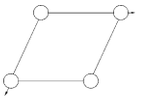
Table 9.1.7.1. *Two-dimensional Bravais lattices*

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

* The symbols for Bravais lattices were adopted by the International Union of Crystallography in 1985; *cf.* de Wolff *et al.* (1985).
† $\boldsymbol{P}(c) = \frac{1}{2}(11/\bar{1}1)$.

obtained from each other by the process of centring'. As a consequence, different Bravais types of the same [crystal] family (*cf.* Section 8.1.4) differ in their centring mode. Thus, the Bravais types may be described by a lower-case letter designating the crystal family and an upper-case letter designating the centring mode. The relations between the point groups of the lattices and the crystal families are shown in Table 9.1.4.1. Since the hexagonal and rhombohedral Bravais types belong to the same crystal family, the rhombohedral lattice is described by hR, h indicating the family and R the centring type. This nomenclature was adopted for the 1969 reprint (*IT* 1969) of *IT* (1952) and for *Structure Reports* since 1975 (*cf.* Trotter, 1975).

9.1.7. Description of Bravais lattices

In Fig. 9.1.7.1, conventional cells for the 14 three-dimensional Bravais lattices are illustrated.

In Tables 9.1.7.1 and 9.1.7.2, the two- and three-dimensional Bravais lattices are described in detail. For each entry, the tables contain conditions that must be fulfilled by the lattice parameters and the metric tensor. These conditions are given with respect to two different basis systems, first the conventional basis related to symmetry, second a special primitive basis (see below). In columns 2 and 3, basis vectors not required by symmetry to be of the same length are designated by different letters. Columns 4 and 5 contain the metric tensors for the two related bases. Column 6 shows the relations between the components of the two tensors.

The last columns of Tables 9.1.7.1 and 9.1.7.2 show parallel projections of the appropriate conventional unit cells. Among the different possible choices of the primitive basis, as discussed in Sections 9.1.1–9.1.5, the special primitive basis mentioned above is obtained according to the following rules:

(i) For each type of centring, only one transformation matrix $\boldsymbol{P}$ is used to obtain the primitive cell as given in Tables 9.1.7.1 and 9.1.7.2. The transformation obeys equation (9.1.1.1).

(ii) Among the different possible transformations, those are preferred which result in a metric tensor with simple relations among its components, as defined in Tables 9.1.7.1 and 9.1.7.2.

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 symmetrically 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.

9.1.8. Delaunay reduction

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.* Chapter 9.3) have shown the common root of both crystallographic approaches. As in Chapters 9.2 and 9.3 the Niggli reduction will be discussed in detail, 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

$$\mathbf{b}_i \cdot \mathbf{b}_k \ (1 \le i < k \le n+1)$$

Table 9.1.7.2. *Three-dimensional Bravais lattices*

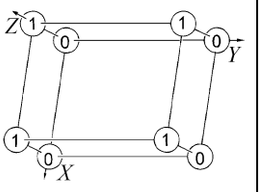
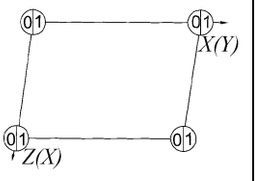
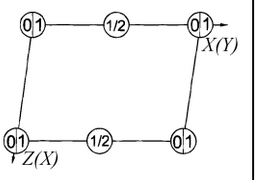
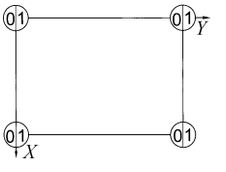
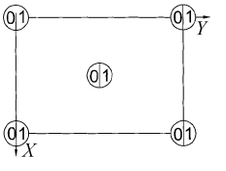
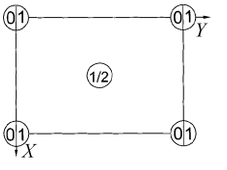
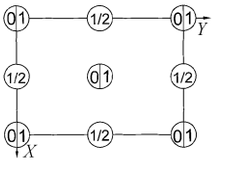
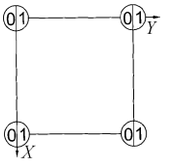
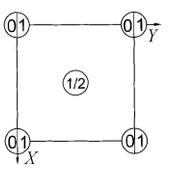
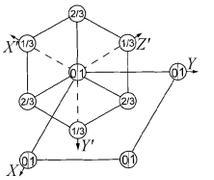
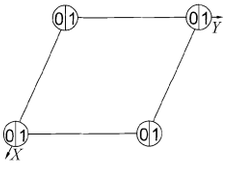
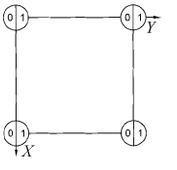
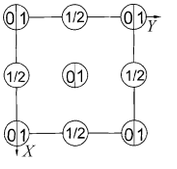
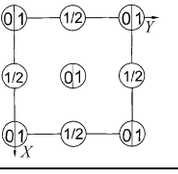
Bravais lattice*	Lattice parameters		Metric tensor			Projections
	Conventional	Primitive	Conventional	Primitive/transf.†	Relations of the components	
aP	a, b, c α, β, γ	a, b, c α, β, γ	$\begin{matrix} g_{11} & g_{12} & g_{13} \\ & g_{22} & g_{23} \\ & & g_{33} \end{matrix}$	$\begin{matrix} g_{11} & g_{12} & g_{13} \\ & g_{22} & g_{23} \\ & & g_{33} \end{matrix}$		
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, b, c $\beta, \alpha = \gamma = 90°$	$a_1 = a_2, c$ $\gamma, \alpha = \beta$	$\begin{matrix} g_{11} & 0 & g_{13} \\ & g_{22} & 0 \\ & & g_{33} \end{matrix}$	$\boldsymbol{P}(C)$ $\begin{matrix} g'_{11} & g'_{12} & g'_{13} \\ & g'_{11} & g'_{13} \\ & & g_{33} \end{matrix}$	$g'_{11} = \frac{1}{4}(g_{11} + g_{22})$ $g'_{12} = \frac{1}{4}(g_{11} - g_{22})$ $g'_{13} = \frac{1}{2} g_{13}$ $g_{11} = 2(g'_{11} + g'_{12})$ $g_{22} = 2(g'_{11} - g'_{12})$ $g_{13} = 2g'_{13}$	
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, b, c $\alpha = \beta = \gamma = 90°$	$a_1 = a_2, c$ $\gamma, \alpha = \beta = 90°$	$\begin{matrix} g_{11} & 0 & 0 \\ & g_{22} & 0 \\ & & g_{33} \end{matrix}$	$\boldsymbol{P}(C)$ $\begin{matrix} g'_{11} & g'_{12} & 0 \\ & g'_{11} & 0 \\ & & g_{33} \end{matrix}$	$g'_{11} = \frac{1}{4}(g_{11} + g_{22})$ $g'_{12} = \frac{1}{4}(g_{11} - g_{22})$ $g_{11} = 2(g'_{11} + g'_{12})$ $g_{22} = 2(g'_{11} - g'_{12})$	
oI	a, b, c $\alpha = \beta = \gamma = 90°$	$a_1 = a_2 = a_3$ α, β, γ $\cos\alpha + \cos\beta + \cos\gamma = -1$	$\begin{matrix} g_{11} & 0 & 0 \\ & g_{22} & 0 \\ & & g_{33} \end{matrix}$	$\boldsymbol{P}(I)$ $\begin{matrix} -\tilde{g} & g'_{12} & g'_{13} \\ & -\tilde{g} & g'_{23} \\ & & -\tilde{g} \end{matrix}$ $\tilde{g} = g'_{12} + g'_{13} + g'_{23}$	$g'_{12} = \frac{1}{4}(-g_{11} - g_{22} + g_{33})$ $g'_{13} = \frac{1}{4}(-g_{11} + g_{22} - g_{33})$ $g'_{23} = \frac{1}{4}(g_{11} - g_{22} - g_{33})$ $g_{11} = -2(g'_{12} + g'_{13})$ $g_{22} = -2(g'_{12} + g'_{23})$ $g_{33} = -2(g'_{13} + g'_{23})$	
oF		a, b, c α, β, γ $\cos\alpha = \dfrac{-a^2 + b^2 + c^2}{2bc}$ $\cos\beta = \dfrac{a^2 + b^2 + c^2}{2ac}$ $\cos\gamma = \dfrac{a^2 + b^2 - c^2}{2ab}$		$\boldsymbol{P}(F)$ $\begin{matrix} \tilde{g}_1 & g'_{12} & g'_{13} \\ & \tilde{g}_2 & g'_{23} \\ & & \tilde{g}_3 \end{matrix}$ $\tilde{g}_1 = g'_{12} + g'_{13}$ $\tilde{g}_2 = g'_{12} + g'_{23}$ $\tilde{g}_3 = g'_{13} + g'_{23}$	$g'_{12} = \frac{1}{4} g_{33}$ $g'_{13} = \frac{1}{4} g_{22}$ $g'_{23} = \frac{1}{4} g_{11}$ $g_{11} = 4g'_{23}$ $g_{22} = 4g'_{13}$ $g_{33} = 4g'_{12}$	

Table 9.1.7.2. *Three-dimensional Bravais lattices* (*cont.*)

Bravais lattice*	Lattice parameters		Metric tensor			Projections
	Conventional	Primitive	Conventional	Primitive/transf.†	Relations of the components	
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		$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma = 60°$		$\boldsymbol{P}(F)$ $\begin{matrix} g'_{11} & \frac{1}{2}g'_{11} & \frac{1}{2}g'_{11} \\ & g'_{11} & \frac{1}{2}g'_{11} \\ & & g'_{11} \end{matrix}$	$g'_{11} = \frac{1}{2}g_{11}$ $g_{11} = 2g'_{11}$	

* See footnote to Table 9.1.7.1. Symbols in parentheses are standard symbols, see Table 2.1.2.1.
† $\boldsymbol{P}(C) = \frac{1}{2}(110/\bar{1}10/002), \boldsymbol{P}(I) = \frac{1}{2}(\bar{1}\bar{1}1/1\bar{1}1/11\bar{1}), \boldsymbol{P}(F) = \frac{1}{2}(011/101/110), \boldsymbol{P}(R) = \frac{1}{3}(\bar{1}2\bar{1}/\bar{2}11/111)$.

Table 9.1.8.1. *The 24 'Symmetrische Sorten'*

In the centred monoclinic lattices, the set $\{\mathbf{a}, \mathbf{c}, \mathbf{a}+\mathbf{c}\} = \{\mathbf{p}, \mathbf{q}, \mathbf{r}\}$ of the three shortest vectors in the **ac** plane is used to describe the metrical conditions. These vectors are renamed according to their relation to the projection of the centring point in the **ac** plane: **p** designates the vector that crosses the projection of the centring point, **q** is the shorter one of the two others and **r** labels the third one.

Delaunay symbol	Bravais type	Metrical conditions (parameters of conventional cells)	Voronoi type	Notation of the scalar products according to equation (9.1.8.1)						Transformation matrix $\boldsymbol{P}$
				12	13	14	23	24	34	
*K*1	*cI*	–	I	12	12	12	12	12	12	011/101/110
*K*2	*cF*	–	III	0	13	13	13	13	0	$1\bar{1}1/111/002$
*K*3	*cP*	–	V	0	0	14	14	14	0	100/001/011
				0	0	14	0	14	14	100/010/001
H	*hP*	–	IV	12	0	12	0	12	34	100/010/001
*R*1	*hR*	$2c^2 < 3a^2$	I	12	12	14	12	14	14	$101/\bar{1}11/0\bar{1}1$
*R*2	*hR*	$2c^2 > 3a^2$	III	0	13	13	13	24	0	101/003/012
*Q*1	*tI*	$c^2 < 2a^2$	I	12	13	13	13	13	12	011/101/110
*Q*2	*tI*	$c^2 > 2a^2$	II	0	13	13	13	13	34	101/011/002
*Q*3	*tP*	–	V	0	0	14	0	14	34	100/010/001
				0	0	14	14	24	0	100/001/011
				0	0	14	23	0	23	001/110/010
*O*1	*oF*	–	I	12	13	13	13	13	34	$1\bar{1}1/111/002$
*O*2	*oI*	$a^2+b^2 > c^2$	I	12	13	14	14	13	12	011/101/110
*O*3	*oI*	$a^2+b^2 < c^2$	II	0	13	13	23	23	34	101/011/002
*O*4	*oI*	$a^2+b^2=c^2$	III	0	13	14	14	13	0	011/101/110
				0	13	13	23	23	0	101/011/002
*O*5	*o*(*AB*)*C*	–	IV	12	0	14	0	12	34	200/110/001
				12	0	14	0	14	34	$110/\bar{1}10/001$
*O*6	*oP*	–	V	0	0	14	0	24	34	100/010/001
				0	0	14	23	24	0	100/001/011
*M*1	*m*(*AC*)*I*	$b^2 > p^2$	I	12	13	14	13	14	34	$\bar{1}10/\bar{1}\bar{1}0/\bar{1}01$
*M*2	*m*(*AC*)*I*	$p^2 > b^2 > r^2-q^2$	I	12	13	14	14	13	34	$01\bar{1}/110/10\bar{1}$
*M*3	*m*(*AC*)*I*	$r^2-q^2 > b^2$	II	0	13	14	23	23	34	$\bar{1}01/\bar{1}10/\bar{2}00$
*M*4	*m*(*AC*)*I*	$b^2=p^2$	II	0	13	14	14	13	34	$01\bar{1}/110/10\bar{1}$
				0	13	14	13	14	34	$\bar{1}10/\bar{1}\bar{1}0/\bar{1}01$
*M*5	*m*(*AC*)*I*	$b^2=r^2-q^2$	III	0	13	14	23	23	0	$\bar{1}01/\bar{1}10/\bar{2}00$
				0	13	14	23	13	0	$10\bar{1}/1\bar{1}0/0\bar{1}\bar{1}$
*M*6	*mP*	–	IV	0	13	14	0	24	34	100/010/001
*T*1	*aP*	–	I	12	13	14	23	24	34	100/010/001
*T*2	*aP*	–	II	0	13	14	23	24	34	100/010/001
*T*3	*aP*	–	III	0	13	14	23	24	0	100/010/001

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

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

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, $\alpha = 90, \beta = 90.67, \gamma = 90°$.

references