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9.1. Bases, lattices, Bravais lattices and other classifications

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9.1.1. Description and transformation of bases

In three dimensions, a coordinate system is defined by an origin and a basis consisting of three non-coplanar vectors. The lengths a, b, c of the basis vectors **a**, **b**, **c** and the intervector angles $\alpha = \angle(\mathbf{b},\mathbf{c})$, $\beta = \angle(\mathbf{c},\mathbf{a})$, $\gamma = \angle(\mathbf{a},\mathbf{b})$ are called the *metric parameters*. In n dimensions, the lengths are designated a_i and the angles α_{ik}, where $1 \leq i < k \leq n$.

Another description of the basis consists of the scalar products of all pairs of basis vectors. The set of these scalar products obeys the rules of covariant tensors of the second rank (see Section 5.1.3). The scalar products may be written in the form of a (3×3) matrix

$$(\mathbf{a}_i \cdot \mathbf{a}_k) = (g_{ik}) = \mathbf{G}; \quad i,k = 1,2,3,$$

which is called the *matrix of the metric coefficients* or the *metric tensor*.

The change from one basis to another is described by a transformation matrix $\boldsymbol{P}$. The transformation of the old basis (**a**, **b**, **c**) to the new basis $(\mathbf{a}',\mathbf{b}',\mathbf{c}')$ is given by

$$(\mathbf{a}',\mathbf{b}',\mathbf{c}') = (\mathbf{a},\mathbf{b},\mathbf{c}) \cdot \boldsymbol{P}.$$

The relation

$$\mathbf{G}' = \boldsymbol{P}^t \cdot \mathbf{G} \cdot \boldsymbol{P} \qquad (9.1.1.1)$$

holds for the metric tensors **G** and **G**′.

9.1.2. Lattices

A three-dimensional lattice can be visualized best as an infinite periodic array of points, which are the termini of the vectors

$$\mathbf{l}_{uvw} = u\mathbf{a} + v\mathbf{b} + w\mathbf{c}, \quad u,v,w \text{ all integers.}$$

The parallelepiped determined by the basis vectors **a**, **b**, **c** is called a (primitive) *unit cell* of the lattice (*cf.* Section 8.1.4), **a**, **b** and **c** are a primitive *basis of the lattice*. The number of possible lattice bases is infinite.

For the investigation of the properties of lattices, appropriate bases are required. In order to select suitable bases (see below), transformations may be necessary (Section 5.1.3). Of the several properties of lattices, only symmetry and some topological aspects are considered in this chapter. Some further properties of lattices are given in Chapter 9.3.

9.1.3. Topological properties of lattices

The treatment of the topological properties is restricted here to the consideration of the neighbourhood of a lattice point. For this purpose, the *domain of influence* (*Wirkungsbereich*, Dirichlet domain, Voronoi domain, Wigner–Seitz cell) (Delaunay, 1933) is introduced. The domain of a particular lattice point consists of all points in space that are closer to this lattice point than to any other lattice point or at most equidistant to it. To construct the domain, the selected lattice point is connected to all other lattice points. The set of planes perpendicular to these connecting lines and passing through their midpoints contains the boundary planes of the domain of influence, which is thus a convex polyhedron. (Niggli and Delaunay used the term 'domain of influence' for the interior of the convex polyhedron only.) Without the use of metrical properties, Minkowski (1897) proved that the maximal number of boundary planes resulting from this construction is equal to $2(2^n - 1)$, where n is the dimension of the space. The minimal number of boundary planes is $2n$. Each face of the polyhedron represents a lattice vector. Thus, the topological, metrical and symmetry properties of infinite lattices can be discussed with the aid of a finite polyhedron, namely the domain of influence (*cf.* Burzlaff & Zimmermann, 1977).

9.1.4. Special bases for lattices

Different procedures are in use to select specific bases of lattices. The reduction procedures employ metrical properties to develop a sequence of basis transformations which lead to a *reduced basis* and *reduced cell* (see Chapter 9.3).

Table 9.1.4.1. *Lattice point-group symmetries*

Two dimensions				
Lattice point group	2	2*mm*	4*mm*	6*mm*
Crystal family*	*m*	*o*	*t*	*h*
	*m*onoclinic (oblique)	*o*rthorhombic (rectangular)	*t*etragonal (square)	*h*exagonal

Three dimensions							
Lattice point group	$C_i \equiv \bar{1}$	$C_{2h} \equiv 2/m$	$D_{2h} \equiv mmm$	$D_{4h} \equiv 4/mmm$	$D_{3d} \equiv \bar{3}m$	$D_{6h} \equiv 6/mmm$	$O_h \equiv m\bar{3}m$
Crystal family*	*a*	*m*	*o*	*t*	*h*		*c*
	*a*northic (triclinic)	*m*onoclinic	*o*rthorhombic	*t*etragonal	*h*exagonal		*c*ubic

* The symbols for crystal families were adopted by the International Union of Crystallography in 1985; *cf.* de Wolff *et al.* (1985).

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Another possibility is to make use of the symmetry properties of lattices. This procedure, with the aid of standardization rules, leads to the *conventional crystallographic basis* and *cell*. In addition to translational symmetry, a lattice possesses point-group symmetry. No crystal can have higher point-group symmetry than the point group of its lattice, which is called *holohedry*. The seven point groups of lattices in three dimensions and the four in two dimensions form the basis for the classification of lattices (Table 9.1.4.1). It may be shown by an algebraic approach (Burckhardt, 1966) or a topological one (Delaunay, 1933) that the arrangement of the symmetry elements with respect to the lattice vectors is not arbitrary but well determined. Taking as basis vectors lattice vectors along important symmetry directions and choosing the origin in a lattice point simplifies the description of the lattice symmetry operations (*cf.* Chapter 12.1). Note that such a basis is not necessarily a (primitive) basis of the lattice (see below). The choice of a basis controlled by symmetry is not always unique; in the monoclinic system, for example, one vector can be taken parallel to the symmetry direction but the other two vectors, perpendicular to it, are not uniquely determined by symmetry.

The choice of conventions for standardizing the setting of a lattice depends on the purpose for which it is used. The several sets of conventions rest on two conflicting principles: symmetry considerations and metric considerations. The following rules (i) to (vii) defining a *conventional basis* are taken from Donnay (1943; Donnay & Ondik, 1973); they deal with the conventions based on symmetry:

(i) Each basis vector is a lattice vector from the origin to the nearest node on the related row. The basis must define a right-handed coordinate system.

(ii) The basis vectors for a *cubic* lattice are parallel to the fourfold axes.

(iii*a*) In a *hexagonal* lattice, one basis vector, parallel to the sixfold axis, is labelled **c**. The remaining two basis vectors are taken along twofold axes and they must include an angle of 120°; from the two possible sets, the shorter vectors are chosen.

(iii*b*) For *rhombohedral* lattices, two descriptions are given in the present edition, as in earlier ones. The first description which gives the conventional cell uses 'hexagonal axes'. In this case, **c** is taken along the threefold axis. The remaining two vectors are chosen along twofold axes including an angle of 120°; they are oriented so that lattice points occur at $2/3, 1/3, 1/3$ and $1/3, 2/3, 2/3$ (obverse setting). The reverse setting $(0, 0, 0; 1/3, 2/3, 1/3; 2/3, 1/3, 2/3)$ is not used in the space-group tables (*cf.* Section 1.2.1, footnote †). The second description uses 'rhombohedral axes': **a**, **b** and **c** are the shortest non-coplanar lattice vectors symmetrically equivalent with respect to the threefold axis.

(iv) In a *tetragonal* lattice, the vector **c** is along the fourfold axis, and **a** and **b** are chosen along twofold axes perpendicular to each other. From the two possible sets, the shorter vectors are chosen.

(v) In an *orthorhombic* lattice, **a**, **b** and **c** must be taken along the twofold axes.

(vi) For *monoclinic* lattices, two 'settings' are given in the present edition. In one setting, the only symmetry direction is labelled **b** (*b*-unique setting). The basis vectors **a** and **c** are chosen to be the shortest two vectors in the net plane perpendicular to **b**, the angle β should be non-acute. This occurs if

$$0 \leq -2\mathbf{a} \cdot \mathbf{c} \leq \min(a^2, c^2). \qquad (9.1.4.1)$$

In the other setting, the symmetry direction is labelled **c** [*c*-unique setting; first introduced in *IT* (1952)]. In this case, **a** and **b** are the shortest two vectors in the net plane perpendicular to **c** and the angle γ should be non-acute. The *b*-unique setting is considered to be the standard setting.

(vii) The reduced basis is used to describe a *triclinic* (= *anorthic*) lattice (*cf.* Chapter 9.3).

The metric parameters of the conventional basis are called *lattice parameters*. For the purpose of identification, additional metric rules have to be employed to make the labelling unique; they can be found in the introduction to *Crystal Data* (Donnay & Ondik, 1973).

When the above rules have been applied, it may occur that not all lattice points can be described by integral coordinates. In such cases, the unit cell contains two, three or four lattice points. The additional points may be regarded as *centrings* of the conventional cell. They have simple rational coordinates. For a conventional basis, the number of lattice points per cell is 1, 2, 3 or 4 (see Tables 9.1.7.1 and 9.1.7.2).

In two dimensions, only two centring types are needed:

p : no centring (primitive);

c : face centred.

In three dimensions, the following centring types are used:

P : no centring (primitive);

I : body centred (*innenzentriert*);

F : all-face centred;

A, B, C : one-face centred, $(\mathbf{b}, \mathbf{c})$ or $(\mathbf{c}, \mathbf{a})$ or $(\mathbf{a}, \mathbf{b})$;

R : hexagonal cell rhombohedrally centred

[see rule (iii*b*) above].

In orthorhombic and monoclinic lattices, some differently centred cells can be transformed into each other without violating the symmetry conditions for the choice of the basis vectors. In these cases, the different centred cells belong to the same *centring mode.* In the orthorhombic case, the three types of one-face-centred cells belong to the same centring mode because the symbol of the cell depends on the labelling of the basis vectors; *C* is usually preferred to *A* and *B* in the standard setting; the centring mode is designated *S* (*seitenflächenzentriert*). In the monoclinic case (*b*-unique setting), *A*, *I* and *C* can be transformed into each other without changing the symmetry direction. *C* is used for the standard setting (*cf.* Section 2.2.3); it represents the centring mode *S*. The vectors **a**, **c** are conventionally chosen as short as the *C*-centring allows so that they need not be the shortest two vectors in their net plane and need not fulfil the inequalities (9.1.4.1).

In some situations, the *I*-centring of the monoclinic conventional cell may be more advantageous. If the vectors **a**, **c** are the shortest ones leading to the centring *I*, they obey the inequalities (9.1.4.1).

9.1.5. Remarks

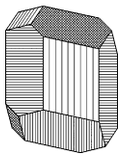
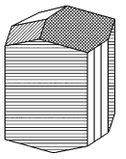
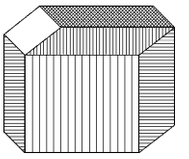
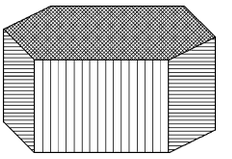
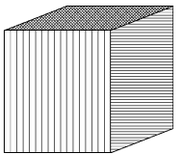
(i) For the handling of special problems such as subgroup relations, it may be convenient to use additional centred cells, *e.g.* a hexagonal cell centred at $2/3, 1/3, 0$ and $1/3, 2/3, 0$, which is called *H*. In this case, rule (iii*a*) above is violated as vectors **a** and **b** are now directed along the second set of twofold axes. Similarly, for tetragonal lattices, *C* may be used instead of *P,* or *F* instead of *I; cf.* Chapter 1.2.

(ii) Readers who have studied Section 8.1.4 may realize that the 'lattice bases' defined here are called 'primitive bases' there and that both 'primitive bases' and 'conventional bases' are special cases of bases used in crystallography.

9.1.6. Classifications

By means of the above-mentioned lattice properties, it is possible to classify lattices according to various criteria. Lattices can be

Table 9.1.6.1. *Representations of the five types of Voronoi polyhedra*

V_I	V_{II}	V_{III}	V_{IV}	V_V
				

subdivided with respect to their topological types of domains, resulting in two classes in two dimensions and five classes in three dimensions. They are called *Voronoi types* (see Table 9.1.6.1). If the classification involves topological *and* symmetry properties of the domains, 24 *Symmetrische Sorten* (Delaunay, 1933) are obtained in three dimensions and 5 in two dimensions. Other classifications consider either the centring type or the point group of the lattice.

The most important classification takes into account both the lattice point-group symmetry and the centring mode (Bravais, 1866). The resulting classes are called *Bravais types of lattices* or, for short, *Bravais lattices*. Two lattices belong to the same Bravais type if and only if they coincide both in their point-group symmetry and in the centring mode of their conventional cells. The Bravais lattice characterizes the translational subgroup of a space group. The number of Bravais lattices is 1 in one dimension, 5 in two dimensions, 14 in three dimensions and 64 in four dimensions. The Bravais lattices may be derived by topological (Delaunay, 1933) or algebraic procedures (Burckhardt, 1966; Neubüser *et al.*, 1971). It can be shown (Wondratschek *et al.*, 1971) that 'all Bravais types of the same crystal family can be

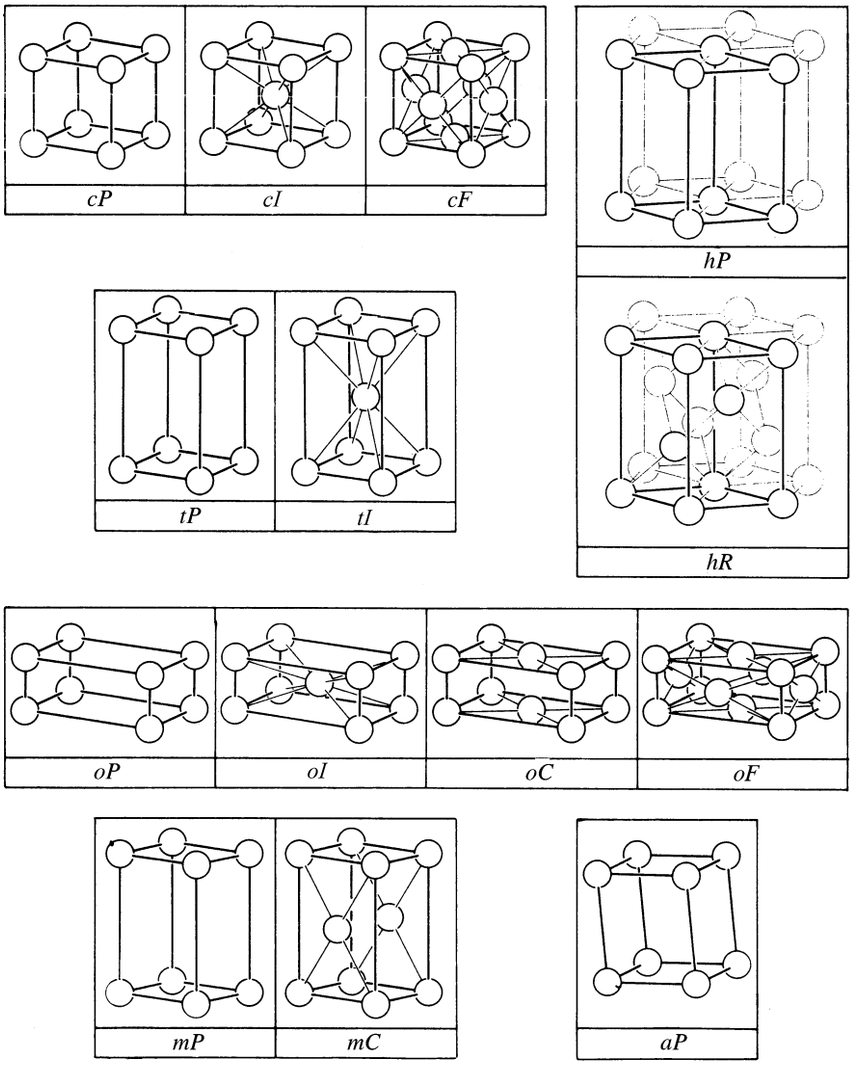
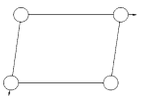
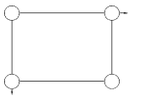
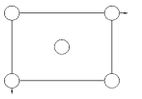
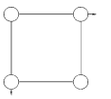
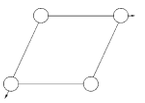


Fig. 9.1.7.1. Conventional cells of the three-dimensional Bravais lattices (for symbols see Table 9.1.7.2).

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	$g_{11}\quad g_{12}$ $\quad\quad g_{22}$	$g_{11}\quad g_{12}$ $\quad\quad g_{22}$		
op	a, b $\gamma = 90°$	a, b $\gamma = 90°$	$g_{11}\quad 0$ $\quad\quad g_{22}$	$g_{11}\quad 0$ $\quad\quad g_{22}$		
oc		$a_1 = a_2, \gamma$ $\boldsymbol{P}(c)$†		$g'_{11}\quad g'_{12}$ $\quad\quad g'_{22}$	$g'_{11} = \frac{1}{4}(g_{11} + g_{22})$ $g'_{12} = \frac{1}{4}(g_{11} - g_{22})$ $g_{11} = 2(g'_{11} + g'_{12})$ $g_{12} = 2(g'_{11} - g'_{12})$	
tp	$a_1 = a_2$ $\gamma = 90°$	$a_1 = a_2$ $\gamma = 90°$	$g_{11}\quad 0$ $\quad\quad g_{11}$	$g_{11}\quad 0$ $\quad\quad g_{11}$		
hp	$a_1 = a_2$ $\gamma = 120°$	$a_1 = a_2$ $\gamma = 120°$	$g_{11}\quad -\frac{1}{2}g_{11}$ $\quad\quad g_{11}$	$g_{11}\quad -\frac{1}{2}g_{11}$ $\quad\quad g_{11}$		

* 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*

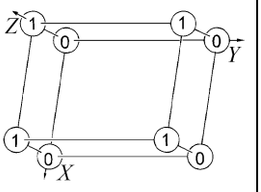
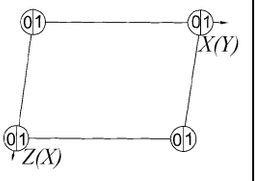
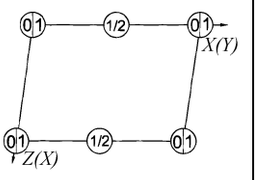
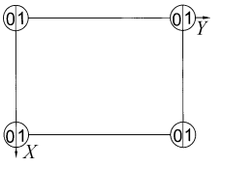
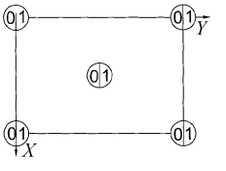
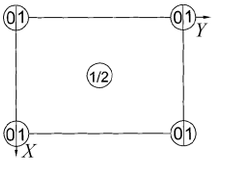
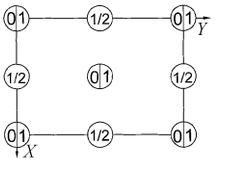
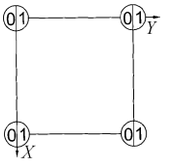
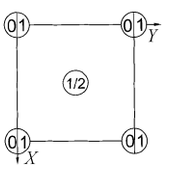
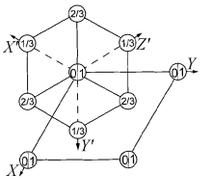
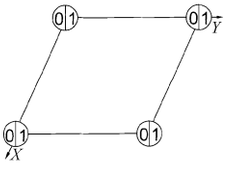
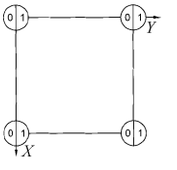
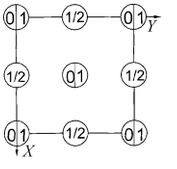
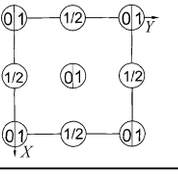
Bravais lattice*	Lattice parameters		Metric tensor			Projections
	Conventional	Primitive	Conventional	Primitive/transf.†	Relations of the components	
aP	a, b, c α, β, γ	a, b, c α, β, γ	$\begin{matrix} g_{11} & g_{12} & g_{13} \\ & g_{22} & g_{23} \\ & & g_{33} \end{matrix}$	$\begin{matrix} g_{11} & g_{12} & g_{13} \\ & g_{22} & g_{23} \\ & & g_{33} \end{matrix}$		
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, $\alpha = 90, \beta = 90.67, \gamma = 90°$.

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