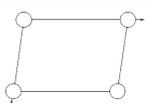
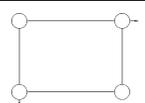
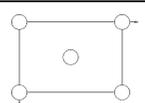
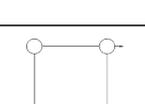
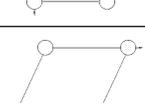


3.1. CRYSTAL LATTICES

Table 3.1.2.1

Two-dimensional Bravais types of lattices

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

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

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 $(\mathbf{b}_i)_{1 \leq i \leq n}$ ($n = 2, 3$). This basis is extended by a vector

$$\mathbf{b}_{n+1} = -(\mathbf{b}_1 + \dots + \mathbf{b}_n).$$

All scalar products

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

are considered. The reduction is performed minimizing the sum

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

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 trans-

formed $\mathbf{b}_i'^2$ is smaller than \sum :

$$\mathbf{b}'_1 = -\mathbf{b}_1, \quad \mathbf{b}'_2 = \mathbf{b}_2, \quad \mathbf{b}'_3 = \mathbf{b}_1 + \mathbf{b}_3 \quad \text{and} \quad \mathbf{b}'_4 = \mathbf{b}_1 + \mathbf{b}_4.$$

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 an 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.