

## 9.1. BASES, LATTICES AND BRAVAIS LATTICES

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	
<i>mp</i>	$a, b$ $\gamma$	$a, b$ $\gamma$	$g_{11} \ g_{12}$ $g_{22}$	$g_{11} \ g_{12}$ $g_{22}$		
<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>		$a_1 = a_2, \gamma$ $\mathbf{P}(c)^\dagger$		$g'_{11} \ g'_{12}$ $g'_{22}$	$g'_{11} = \frac{1}{4}(g_{11} + g_{22})$ $g'_{12} = \frac{1}{4}(g_{11} - g_{22})$ $g_{11} = 2(g'_{11} + g'_{12})$ $g_{12} = 2(g'_{11} - g'_{12})$	
<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 lattices were adopted by the International Union of Crystallography in 1985; cf. de Wolff *et al.* (1985).

$\dagger \mathbf{P}(c) = \frac{1}{2}(11/\bar{1}1)$ .

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

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

All scalar products

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