Table 3.1.1.1
Lattice point-group symmetries

(*a*) 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

(*b*) 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).

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

(iii*a*) In a *hexagonal* lattice, the basis vector parallel to the sixfold axis is labelled **c**. The remaining two basis vectors are taken along equivalent 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 results in the conventional cell uses 'hexagonal axes'. In this case, **c** is taken along the threefold axis. The remaining two vectors are chosen along equivalent twofold axes, which include 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.* the second footnote to Table 2.1.1.2). The second description uses 'rhombohedral axes': **a**, **b** and **c** are the shortest three non-coplanar lattice vectors symmetry-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 equivalent 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 three 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

$$0 \leq -2\mathbf{a} \cdot \mathbf{c} \leq \min(a^2, c^2). \qquad (3.1.1.3)$$

In the other setting, the symmetry direction is labelled **c** [*c*-unique setting; first introduced in *International Tables for X-ray Crystallography* (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.* Section 3.1.4).

The metric parameters of the conventional basis are called *lattice parameters*. For the purpose of identification, additional metric rules are to be applied 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 3.1.2.1 and 3.1.2.2).

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, either (**b**, **c**) or (**c**, **a**) or (**a**, **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 only on the labelling of the basis vectors; *C* is usually preferred to *A* and *B* as the standard setting; the centring mode is designated *S* (*seitenflächenzentriert*). In the monoclinic case (*b*-unique setting), *A*, *I* and *C* may occur if the basis is chosen according to rule (vi). They can be transformed into each other without changing the symmetry direction. *C* is used for the standard setting (*cf.* Section 2.1.1.2); 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 (3.1.1.3).

3.1.1.5. Remarks

(i) For the handling of special problems such as subgroup relations, it may be convenient to use additional types of 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 equivalent twofold axes. Similarly, for tetragonal

lattices, *C* may be used instead of *P*, or *F* instead of *I*; *cf.* Sections 1.5.4 and 2.1.1.2.

(ii) Readers who have studied Chapter 1.3 may realize that the 'lattice bases' defined here are also called 'primitive bases' and that both 'primitive bases' and 'conventional bases' are special cases of bases used in crystallography.

3.1.2. Bravais types of lattices and other classifications

By H. Burzlaff and H. Zimmermann

3.1.2.1. Classifications

By means of the above-mentioned lattice properties, it is possible to classify lattices according to various criteria. Lattices can be 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*. 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 obtained from each other by the process of centring'. As a consequence, different Bravais types of the same crystal family (*cf.* Section 1.3.4) 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 3.1.1.1. 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 of *International Tables for X-ray Crystallography* (1952) and for *Structure Reports* since 1975 (*cf.* Trotter, 1975).

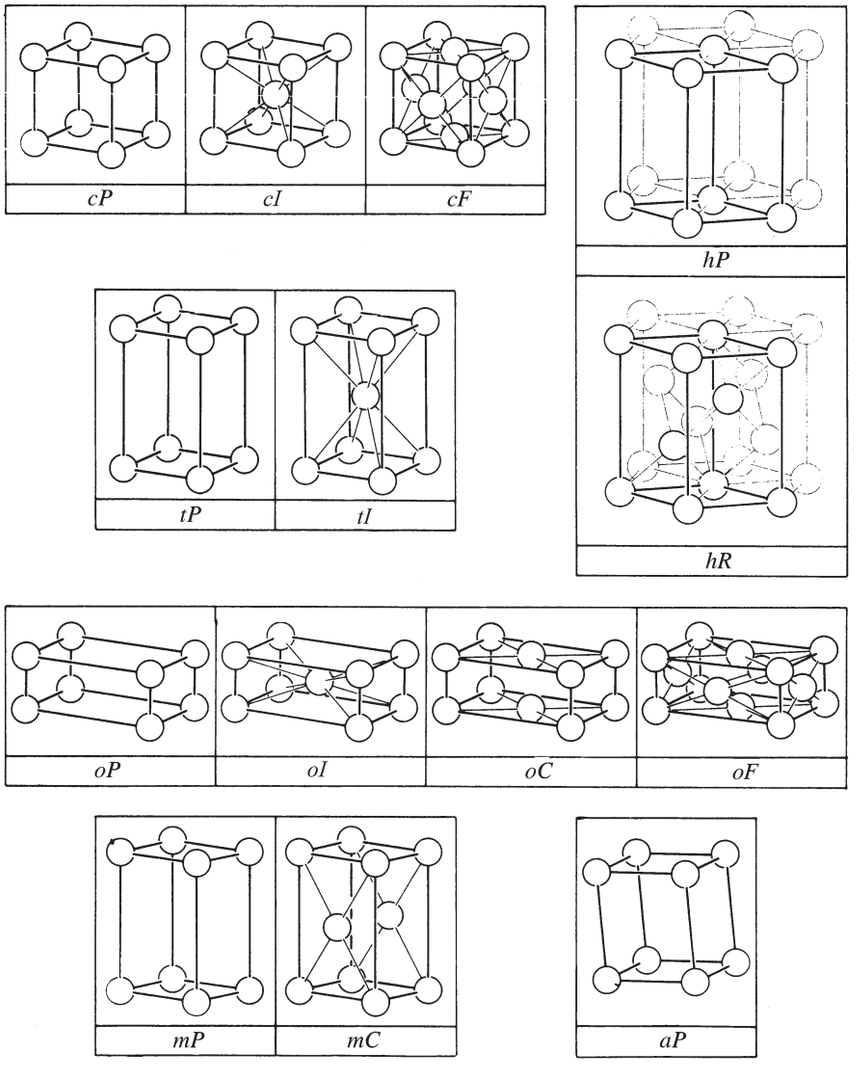

Figure 3.1.2.1
Conventional cells of the three-dimensional Bravais types of lattices (for symbols see Table 3.1.2.2).

3.1.2.2. Description of Bravais types of lattices

In Fig. 3.1.2.1, conventional cells for the 14 three-dimensional Bravais types of lattices are illustrated.

In Tables 3.1.2.1 and 3.1.2.2, the two- and three-dimensional Bravais types of 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 3.1.2.1 and 3.1.2.2 show parallel projections of the appropriate conventional unit cells. Among the different possible choices of the primitive basis, as discussed in Section 3.1.1, 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 3.1.2.1 and 3.1.2.2. The transformation obeys equation (3.1.1.2).

(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 3.1.2.1 and 3.1.2.2.