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

references