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