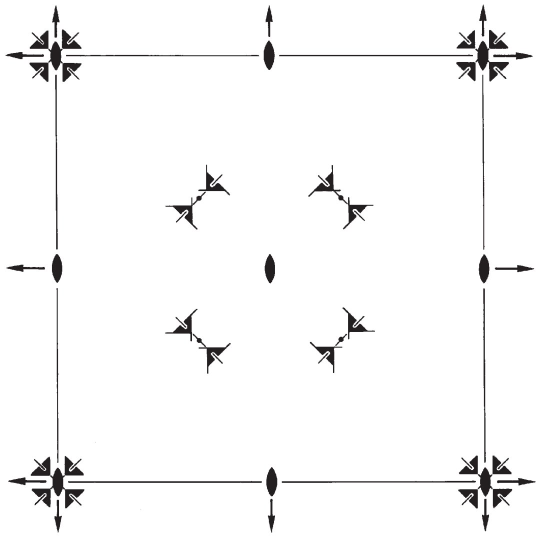

Figure 1.5.4.1
Symmetry-element diagram for space group *P*23 (195).

The analysis illustrates that the combination of the twofold rotation $2\ x, x, 0$ with *I*-centring translations gives rise to symmetry elements of rotation and of screw rotation type (*cf.* Table 1.5.4.2).

Example 5

Let $W = x, y, \bar{z}$ be a reflection $m\ x, y, 0$ with the c axis normal to the reflection plane. An *F*-centred lattice contains a centring translation $t(\frac{1}{2}, \frac{1}{2}, 0)$ and the composition of W with this translation is an n glide, since the intrinsic translation part of $W' = x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$ is $\boldsymbol{w}'_g = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix}$ and consequently the location part is $\boldsymbol{w}'_l = \boldsymbol{o}$. The symmetry operation W' is thus an n glide with the plane $x, y, 0$ as geometric element. However, since the intrinsic translation part $\boldsymbol{w}_g$ is a lattice vector, W and W' are coplanar equivalents and belong to the element set of the same symmetry element, which is a reflection plane.

The composition of $W = x, y, \bar{z}$ with $t(0, \frac{1}{2}, \frac{1}{2})$ is a b glide, because $W' = x, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ has intrinsic translation part $\boldsymbol{w}'_g = \begin{pmatrix} 0 \\ \frac{1}{2} \\ 0 \end{pmatrix}$. The location part is $\boldsymbol{w}'_l = \begin{pmatrix} 0 \\ 0 \\ \frac{1}{2} \end{pmatrix}$ and since $(\boldsymbol{I} - \boldsymbol{W})\boldsymbol{p} = \boldsymbol{w}'_l$ for $\boldsymbol{p} = \begin{pmatrix} 0 \\ 0 \\ \frac{1}{4} \end{pmatrix}$, the geometric element of this glide reflection is the plane $x, y, \frac{1}{4}$. Likewise, the composition $W' = x + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$ of W with $t(\frac{1}{2}, 0, \frac{1}{2})$ is an a glide with the same plane $x, y, \frac{1}{4}$ as geometric element. The two symmetry operations $b\ x, y, \frac{1}{4}$ and $a\ x, y, \frac{1}{4}$, differing only by the lattice vector $(-\frac{1}{2}, \frac{1}{2}, 0)$ in their translation parts, are coplanar equivalents and belong to the element set of an *e*-glide plane (*cf.* Section 1.2.3 for an introduction to *e*-glide notation).

1.5.4.2. Synoptic table of the plane groups

The possible plane-group symbols are listed in Table 1.5.4.3. Two cases of multiple cells are included in addition to the standard cells, namely the c centring in the square system and the h centring in the hexagonal system. The c centring is defined by

$$\mathbf{a}' = \mathbf{a} \mp \mathbf{b};\ \ \mathbf{b}' = \pm\mathbf{a} + \mathbf{b}$$

with centring points at 0, 0 and $\frac{1}{2}, \frac{1}{2}$. The triple h cell is defined by

$$\mathbf{a}' = \mathbf{a} - \mathbf{b};\ \ \mathbf{b}' = \mathbf{a} + 2\mathbf{b}$$

with centring points at 0, 0; $\frac{2}{3}, \frac{1}{3}$ and $\frac{1}{3}, \frac{2}{3}$. The glide lines g directly listed under the mirror lines m in the extended and multiple cell symbols indicate that the two symmetry elements are parallel and alternate in the perpendicular direction.

1.5.4.3. Synoptic table of the space groups

Table 1.5.4.4 gives a comprehensive listing of the possible space-group symbols for various settings and choices of the unit cell. The data are ordered according to the crystal systems. The extended Hermann–Mauguin symbols provide information on the additional symmetry operations generated by the compositions of the symmetry operations with lattice translations. An extended Hermann–Mauguin symbol is a complex multi-line symbol: (i) the first line contains those symmetry operations for which the coordinate triplets are explicitly printed under 'Positions' in the space-group tables in this volume; (ii) the entries of the lines below indicate the additional symmetry operations generated by the compositions of the symmetry operations of the first line with lattice translations. For example, for *A*-, *B*-, *C*- and *I*-centred space groups, the entries of the second line of the two-line extended symbol denote the symmetry operations generated by combinations with the corresponding centring translations.[3]

In the triclinic system the corresponding symbols do not depend on any space direction. Therefore, only the two standard symbols *P*1 (1) and $P\bar{1}$ (2) are listed. One should, however, bear in mind that in some circumstances it might be more appropriate to use a centred cell for comparison purposes, *e.g.* following a phase transition resulting from a temperature, pressure or composition change.

The monoclinic and orthorhombic systems present the largest number of alternatives owing to various settings and cell choices. In the monoclinic system, three choices of unique axis can occur, namely b, c and a. In each case, two permutations of the other axes are possible, thus yielding six possible settings given in terms of three pairs, namely $\mathbf{a\underline{b}c}$ and $\mathbf{c\underline{b}\bar{a}}$, $\mathbf{ab\underline{c}}$ and $\mathbf{ba\underline{\bar{c}}}$, $\mathbf{\underline{a}bc}$ and $\mathbf{\underline{\bar{a}}cb}$. The unique axes are underlined and the negative sign, placed over the letter, maintains the correct handedness of the reference system. The three possible cell choices indicated in Fig. 1.5.3.1 increase the number of possible symbols by a factor of three, thus yielding 18 different cases for each monoclinic space group, except for five cases, namely *P*2 (3), $P2_1$ (4), *Pm* (6), *P*2/*m* (10) and $P2_1/m$ (11) with only six variants.

In monoclinic *P* lattices, the symmetry operations along the symmetry direction are always unique. Here again, as in the plane groups, the cell centrings give rise to additional entries in the extended Hermann–Mauguin symbols. Consider, for example, the data for monoclinic *P*12/*m*1 (10), *C*12/*m*1 (12) and *C*12/*c*1 (15) in Table 1.5.4.4. For *P*12/*m*1 and its various settings there is only one line, which corresponds to the full Hermann–Mauguin symbols; these contain only rotations 2 and reflections *m*. The first line for *C*12/*m*1 is followed by a second line, the first entry of which is the symbol $2_1/a$, because 2_1 screw rotations and a glide reflections also belong to this space group. Similarly, in *C*12/*c*1

[3] After the introduction of the *e*-glide convention and the symmetry-element interpretation of the characters of the Hermann–Mauguin symbols (de Wolff *et al.*, 1992), the tabulated data for the extended symbols were partially modified by introducing the *e*-glide notation in the symbols of only some of the groups [*cf.* Table 4.3.2.1 of the fifth edition of *IT* A (2002)]. In contrast to the fifth edition, in Table 1.5.4.4 extended symbols similar to those that can be found in the first four editions of *IT* A have been reinstated.