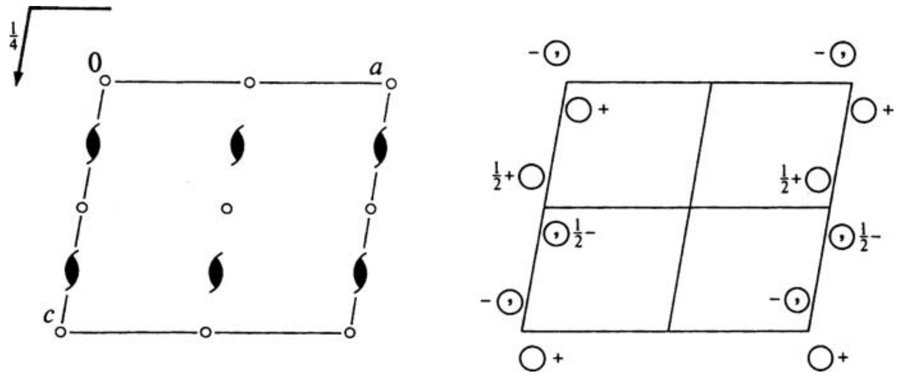

Figure 1.4.2.6
Symmetry-element diagram (left) and general-position diagram (right) for the space group $P2_1/c$, No. 14 (unique axis b, cell choice 1).

The thin lines outlining the projection are the traces of the side planes of the unit cell.

Detailed explanations of the diagrams of space groups are found in Section 2.1.3.6. In this section, after a very brief introduction to the diagrams, we will focus mainly on certain important but very often overlooked features of the diagrams.

Symmetry-element diagram

The graphical symbols of the symmetry elements used in the diagrams are explained in Section 2.1.2. The heights along the projection direction above the plane of the diagram are indicated for rotation or screw axes and mirror or glide planes parallel to the projection plane, for rotoinversion axes and inversion centres. The heights (if different from zero) are given as fractions of the shortest translation vector along the projection direction. In Fig. 1.4.2.6 (left) the symmetry elements of $P2_1/c$ (unique axis b, cell choice 1) are represented graphically in a projection of the unit cell along the monoclinic axis **b**. The directions of the basis vectors **c** and **a** can be read directly from the figure. The origin (upper left corner of the unit cell) lies on a centre of inversion indicated by a small open circle. The black lenticular symbols with tails represent the twofold screw axes parallel to **b**. The c-glide plane at height $\frac{1}{4}$ along **b** is shown as a bent arrow with the arrowhead pointing along **c**.

The crystallographic symmetry operations are visualized geometrically by the related symmetry elements. Whereas the symmetry element of a symmetry operation is uniquely defined, more than one symmetry operation may belong to the same symmetry element (*cf.* Section 1.2.3). The following examples illustrate some important features of the diagrams related to the fact that the symmetry-element symbols that are displayed visualize all symmetry operations that belong to the element sets of the symmetry elements.

Examples

(1) *Visualization of the twofold screw rotations of* $P2_1/c$ (Fig. 1.4.2.6). The second coset of the decomposition of $P2_1/c$ with respect to its translation subgroup shown in Table 1.4.2.6 is formed by the infinite set of twofold screw rotations represented by the coordinate triplets $\bar{x}+u_1$, $y+\frac{1}{2}+u_2, \bar{z}+\frac{1}{2}+u_3$ (where u_1, u_2, u_3 are integers). To analyse how these symmetry operations are visualized, it is convenient to consider two special cases:

(i) $u_2 = 0$, *i.e.* $\bar{x}+u_1,\ y+\frac{1}{2},\ \bar{z}+\frac{1}{2}+u_3 = \{2_{010}|u_1, \frac{1}{2}, \frac{1}{2}+u_3\}$; these operations correspond to twofold screw rotations around the infinitely many screw axes parallel to the line $0, y, \frac{1}{4}$, *i.e.* around the lines $u_1/2, y, u_3/2+\frac{1}{4}$. The symbols of the symmetry elements (*i.e.* of the twofold screw axes) located in the unit cell at $0, y, \frac{1}{4}$; $0, y, \frac{3}{4}$; $\frac{1}{2}, y, \frac{1}{4}$; $\frac{1}{2}, y, \frac{3}{4}$ (and the translationally equivalent $1, y, \frac{1}{4}$ and $1, y, \frac{3}{4}$) are shown in the symmetry-element diagram (Fig. 1.4.2.6);

(ii) $u_1 = u_3 = 0$, *i.e.* $\bar{x},\ y+\frac{1}{2}+u_2,\ \bar{z}+\frac{1}{2} = \{2_{010}|0, \frac{1}{2}+u_2, \frac{1}{2}\}$; these symmetry operations correspond to screw rotations around the line $0, y, \frac{1}{4}$ with screw components $\frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \ldots, -\frac{1}{2}, -\frac{3}{2}, -\frac{5}{2}, \ldots$, *i.e.* with a screw component $\frac{1}{2}$ to which all lattice translations parallel to the screw axis are added. These operations, infinite in number, share the same geometric element, *i.e.* they form the element set of the same symmetry element, and geometrically they are represented just by one graphical symbol on the symmetry-element diagrams located exactly at $0, y, \frac{1}{4}$.

(iii) The rest of the symmetry operations in the coset, *i.e.* those with the translation parts $\begin{pmatrix} u_1 \\ \frac{1}{2}+u_2 \\ \frac{1}{2}+u_3 \end{pmatrix}$, are combinations of the two special cases above.

(2) *Inversion centres of* $P2_1/c$ (Fig. 1.4.2.6). The element set of an inversion centre consists of only one symmetry operation, *viz.* the inversion through the point located at the centre. In other words, to each inversion centre displayed on a symmetry-element diagram there corresponds one symmetry operation of inversion. The infinitely many inversions $(-\boldsymbol{I}, \boldsymbol{t}) = \bar{x}+u_1, \bar{y}+u_2, \bar{z}+u_3 = \{\bar{1}|u_1, u_2, u_3\}$ of $P2_1/c$ are located at points $u_1/2$, $u_2/2, u_3/2$. Apart from translational equivalence, there are eight centres located in the unit cell: four at $y = 0$, namely at $0, 0, 0$; $\frac{1}{2}, 0, 0$; $0, 0, \frac{1}{2}$; $\frac{1}{2}, 0, \frac{1}{2}$ and four at height $\frac{1}{2}$ of b. It is important to note that only inversion centres at $y = 0$ are indicated on the diagram.

A similar rule is applied to all pairs of symmetry elements of the same type (such as *e.g.* twofold rotation axes, planes *etc.*) whose heights differ by $\frac{1}{2}$ of the shortest lattice direction along the projection direction. For example, the c-glide plane symbol in Fig. 1.4.2.6 with the fraction $\frac{1}{4}$ next to it represents not only the c-glide plane located at height $\frac{1}{4}$ but also the one at height $\frac{3}{4}$.

(3) *Glide reflections visualized by mirror planes*. As discussed in Section 1.2.3, the element set of a mirror or glide plane consists of a defining operation and all its coplanar equivalents (*cf.* Table 1.2.3.1). The corresponding symmetry element is a mirror plane if among the infinite set of the coplanar glide reflections there is one with zero glide vector. Thus, the symmetry element is a mirror plane and