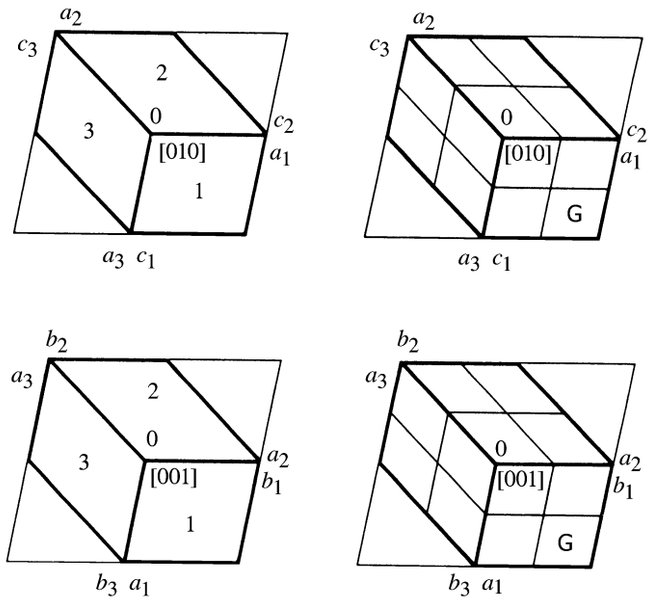

Fig. 2.2.6.4. Monoclinic space groups, cell choices 1, 2, 3. Upper pair of diagrams: setting with unique axis *b*. Lower pair of diagrams: setting with unique axis *c*. The numbers 1, 2, 3 within the cells and the subscripts of the labels of the axes indicate the cell choice (*cf.* Section 2.2.16). The unique axis points upwards from the page.

standard setting, **a**, **b**, **c**, into those of the setting considered. For instance, the setting symbol **cab** stands for the cyclic permutation

$$\mathbf{a}' = \mathbf{c}, \quad \mathbf{b}' = \mathbf{a}, \quad \mathbf{c}' = \mathbf{b}$$

or

$$(\mathbf{a}'\mathbf{b}'\mathbf{c}') = (\mathbf{abc})\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} = (\mathbf{cab}),$$

where $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$ is the new set of basis vectors. An interchange of two axes reverses the handedness of the coordinate system; in order to keep the system right-handed, each interchange is accompanied by the reversal of the sense of one axis, *i.e.* by an element $\bar{1}$ in the transformation matrix. Thus, $\mathbf{ba\bar{c}}$ denotes the transformation

$$(\mathbf{a}'\mathbf{b}'\mathbf{c}') = (\mathbf{abc})\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix} = (\mathbf{ba\bar{c}}).$$

The six orthorhombic settings correspond to six Hermann–Mauguin symbols which, however, need not all be different; *cf.* Table 2.2.6.1.*

In the earlier (1935 and 1952) editions of *International Tables*, only one setting was illustrated, in a projection along *c*, so that it was usual to consider it as the 'standard setting' and to accept its cell edges as crystal axes and its space-group symbol as 'standard Hermann–Mauguin symbol'. In the present edition, however, *all six* orthorhombic settings are illustrated, as explained below.

The three projections of the symmetry elements can be interpreted in two ways. First, in the sense indicated above, that is, as different projections of a *single* (standard) setting of the space group, with the projected basis vectors **a**, **b**, **c** labelled as in Fig. 2.2.6.5. Second, each one of the three diagrams can be considered as the projection along $\mathbf{c}'$ of either one of *two different* settings: one setting in which $\mathbf{b}'$ is horizontal and one in which $\mathbf{b}'$ is vertical ($\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$ refer to the setting under consideration). This second interpretation is used to illustrate in the same figure the space-group symbols corresponding to these two settings. In order to view these projections in conventional orientation ($\mathbf{b}'$ horizontal, $\mathbf{a}'$ vertical, origin in the upper left corner, projection down the positive $\mathbf{c}'$ axis), the setting with $\mathbf{b}'$ horizontal can be inspected directly with the figure upright; hence, the corresponding space-group symbol is printed above the projection. The other setting with $\mathbf{b}'$ vertical and $\mathbf{a}'$ horizontal, however, requires turning the figure over 90°, or looking at it from the side; thus, the space-group symbol is printed at the left, and it runs upwards.

The 'setting symbols' for the six settings are attached to the three diagrams of Fig. 2.2.6.6, which correspond to those of Fig. 2.2.6.5. In the orientation of the diagram where the setting symbol is read in the usual way, $\mathbf{a}'$ is vertical pointing downwards, $\mathbf{b}'$ is horizontal pointing to the right, and $\mathbf{c}'$ is pointing upwards from the page. Each setting symbol is printed in the position that in the space-group tables is actually occupied by the corresponding full Hermann–Mauguin symbol. The changes in the space-group symbol that are

* A space-group symbol is invariant under sign changes of the axes; *i.e.* the same symbol applies to the right-handed coordinate systems $\mathbf{abc}$, $\mathbf{a\bar{b}\bar{c}}$, $\mathbf{\bar{a}b\bar{c}}$, $\mathbf{\bar{a}\bar{b}c}$ and the left-handed systems $\mathbf{\bar{a}\bar{b}\bar{c}}$, $\mathbf{\bar{a}bc}$, $\mathbf{ab\bar{c}}$, $\mathbf{\bar{a}\bar{b}\bar{c}}$.

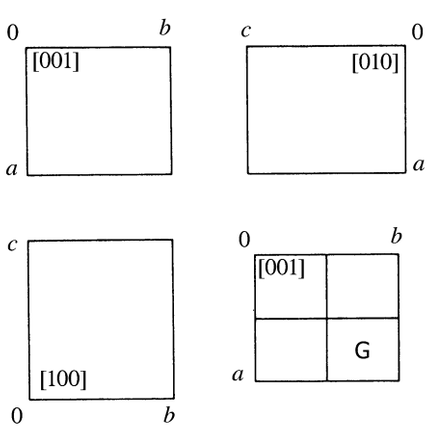

Fig. 2.2.6.5. Orthorhombic space groups. Diagrams for the 'standard setting' as described in the space-group tables (G = general-position diagram).

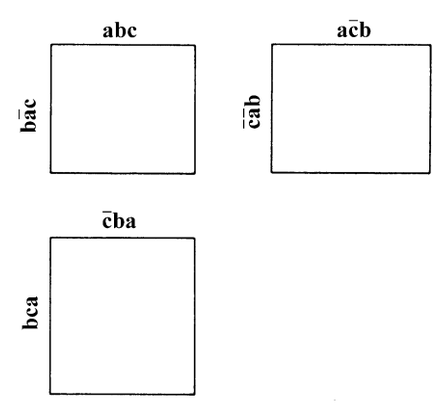

Fig. 2.2.6.6. Orthorhombic space groups. The three projections of the symmetry elements with the six setting symbols (see text). For setting symbols printed vertically, the page has to be turned clockwise by 90° or viewed from the side. Note that in the actual space-group tables instead of the setting symbols the corresponding full Hermann–Mauguin space-group symbols are printed.

references