Summarizing, the types of symmetry operations $\mathcal{W} = (\boldsymbol{W}, \boldsymbol{w})$ and their symmetry elements can be identified as follows:

(i) Decompose the translation part $\boldsymbol{w}$ as $\boldsymbol{w} = \boldsymbol{w}_g + \boldsymbol{w}_l$, where $\boldsymbol{w}_g$ and $\boldsymbol{w}_l$ are mutually perpendicular and the intrinsic translation part $\boldsymbol{w}_g$ is fixed by the linear part $\boldsymbol{W}$ of $\mathcal{W}$.

(ii) Determine a shift of origin $\boldsymbol{p}$ such that $(\boldsymbol{I} - \boldsymbol{W})\boldsymbol{p} = \boldsymbol{w}_l$, *i.e.* such that $\boldsymbol{p}$ is a fixed point of the reduced operation $(\boldsymbol{W}, \boldsymbol{w}_l)$.

(iii) For the correct determination of the defining operation of the symmetry element it may be necessary to reduce the intrinsic translation part $\boldsymbol{w}_g$ by a lattice translation in the fixed space of $\boldsymbol{W}$, thus yielding a coplanar or coaxial equivalent symmetry operation.

This analysis allows one to read off the types of the symmetry operations and of the corresponding symmetry elements that occur for the coset $\mathcal{T}\mathcal{W}$ of $\mathcal{W}$. The following two sections provide examples illustrating that in some cases the coset does not contain symmetry operations belonging to symmetry elements of different type, while in others it does.

1.5.4.1.2. *Cosets without additional types of symmetry elements*

In cases where the linear part $\boldsymbol{W}$ of a symmetry operation $\mathcal{W}$ fixes only the origin, all elements in the coset are of the same type. This is due to the fact that the translation part $\boldsymbol{w}$ is decomposed as $\boldsymbol{w}_g = \boldsymbol{o}$ and $\boldsymbol{w}_l = \boldsymbol{w}$. Since $\boldsymbol{W}$ fixes only the origin, $\boldsymbol{I} - \boldsymbol{W}$ is invertible and a fixed point $\boldsymbol{p}$ of the reduced operation $(\boldsymbol{W}, \boldsymbol{w}_l) = (\boldsymbol{W}, \boldsymbol{w})$ can be found, as $\boldsymbol{p} = (\boldsymbol{I} - \boldsymbol{W})^{-1}\boldsymbol{w}$. This situation occurs when $\mathcal{W}$ is an inversion or a three-, four- or sixfold rotoinversion. The element set of the symmetry element of an inversion consists only of this inversion; the element set of a rotoinversion consists of the rotoinversion $\mathcal{W}$ and its inverse $\mathcal{W}^{-1}$ (the latter belonging to a different coset). Therefore, in these cases each symmetry operation in the coset of $\mathcal{W}$ belongs to the element set of a different symmetry element (of the same type, namely an inversion centre or a rotoinversion axis).

Note that the above argument does not apply to twofold rotoinversions, since these are in fact reflections which fix a plane perpendicular to the rotoinversion axis and not only a single point. The following two examples illustrate that translations from a primitive lattice do not give rise to symmetry elements of different type in the cases of either a reflection or glide reflection with normal vector along one of the coordinate axes, or of a rotation or screw rotation with rotation axis along one of the coordinate axes.

Example 1

Let $\mathcal{W} = x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$ be an *n* glide with normal vector along the *c* axis. For the composition of $\mathcal{W}$ with an integral translation $t(u_1, u_2, u_3)$ one obtains a symmetry operation $\mathcal{W}'$ with translation part $\boldsymbol{w}' = \begin{pmatrix} u_1 + \frac{1}{2} \\ u_2 + \frac{1}{2} \\ u_3 \end{pmatrix}$. The decomposition of $\boldsymbol{w}'$ into the intrinsic translation part and the location part gives $\boldsymbol{w}'_g = \begin{pmatrix} u_1 + \frac{1}{2} \\ u_2 + \frac{1}{2} \\ 0 \end{pmatrix}$ and $\boldsymbol{w}'_l = \begin{pmatrix} 0 \\ 0 \\ u_3 \end{pmatrix}$. This shows that the intrinsic translation part is only changed by the lattice vector $\begin{pmatrix} u_1 \\ u_2 \\ 0 \end{pmatrix}$ and hence $\mathcal{W}'$ is a coplanar equivalent of the symmetry operation $\mathcal{W}'' = x + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + u_3$, which is an *n* glide with glide plane normal to the *c* axis and located at $z = u_3/2$. One concludes that $\mathcal{W}$ and $\mathcal{W}'$ belong to symmetry elements of the same type. The same conclusion would in fact remain true in the case of a *C*-centred lattice, since the composition of $\mathcal{W}$ with the centring translation $t(\frac{1}{2}, \frac{1}{2}, 0)$ would simply result in the intrinsic translation part being changed by the centring translation.

Example 2

As an example of a rotation, let $\mathcal{W} = \bar{y}, x, z$ be a fourfold rotation $4^+\ 0, 0, z$ around the *c* axis. Composing $\mathcal{W}$ with the translation $t(u_1, u_2, u_3)$ results in the symmetry operation $\mathcal{W}' = \bar{y} + u_1, x + u_2, z + u_3$ with intrinsic translation part $\boldsymbol{w}'_g = \begin{pmatrix} 0 \\ 0 \\ u_3 \end{pmatrix}$ and location part $\boldsymbol{w}'_l = \begin{pmatrix} u_1 \\ u_2 \\ 0 \end{pmatrix}$. Since we assume a primitive lattice, u_3 is an integer, hence $\mathcal{W}'$ is a coaxial equivalent of the symmetry operation $\mathcal{W}'' = \bar{y} + u_1, x + u_2, z$, which has intrinsic translation part $\boldsymbol{o}$. To locate the geometric element of $\mathcal{W}'$, one notes that for

$$\boldsymbol{W} = \begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

one has

$$(\boldsymbol{I} - \boldsymbol{W})\boldsymbol{p} = \boldsymbol{w}'_l \text{ for } \boldsymbol{p} = \begin{pmatrix} (u_1 - u_2)/2 \\ (u_1 + u_2)/2 \\ 0 \end{pmatrix}.$$

The symmetry operation $\mathcal{W}'$ therefore belongs to the symmetry element of a fourfold rotation with the line $(u_1 - u_2)/2, (u_1 + u_2)/2, z$ as geometric element. This analysis shows that all symmetry operations in the coset $\mathcal{T}\mathcal{W}$ belong to the same type of symmetry element, since for each of these symmetry operations a coaxial equivalent can be found that has zero screw component.

1.5.4.1.3. *Examples with additional types of symmetry elements*

The examples given in the previous section illustrate that in the case of a translation vector perpendicular to the symmetry axis or symmetry plane of a symmetry operation, the intrinsic translation vector remains unchanged and only the location of the geometric element is altered. In particular, composition with such a translation vector results in symmetry operations and symmetry elements of the same type. On the other hand, composition with translations parallel to the symmetry axis or symmetry plane give rise to coaxial or coplanar equivalents, which also belong to the same symmetry element. Combining these two observations shows that for integral translations, only translations along a direction inclined to the symmetry axis or symmetry plane can give rise to additional symmetry elements. For these cases, the additional symmetry operations and their locations are summarized in Table 1.5.4.1.

In space groups with a centred lattice, the translation subgroup contains also translations with non-integral components, and these often give rise to symmetry operations and symmetry elements of different types in the same coset. An overview of additional symmetry operations and their locations that occur due to centring vectors is given in Table 1.5.4.2. In rhombohedral space groups all additional types of symmetry elements occur already as a result of combinations with integral lattice translations (*cf.* Table 1.5.4.1). For this reason, the rhombohedral centring *R* case is not included in Table 1.5.4.2.

In Section 1.4.2.4 the occurrence of glide reflections in a space group of type *P*4*mm* (due to integral translations inclined to a