Bragg intensities in comparison with the untwinned crystals, however, makes a structure determination more difficult.

Type 2: The twin operation does not belong to the Laue class of the crystal. Such twins can occur only in point groups marked by an asterisk in Table 1.3.4.1, *i.e.* in 55 out of the 159 types of space groups mentioned above. If the different twin components occur with equal volumes, the corresponding diffraction pattern shows enhanced symmetry. On the contrary, the reflection conditions are unchanged in comparison to those for a single crystal, except for $Pa\bar{3}$. As a consequence, for 51 out of the 55 space-group types, the derivation of 'possible space groups', as described in *IT* A (1983, Part 3), gives incorrect results. For $P4_2/n$, $I4_1/a$ and $Ia\bar{3}$, the combination of the simulated Laue class of the twin and the (unchanged) extinction symbol does not occur for single crystals. Therefore, the symmetry of these twins can be determined uniquely. In the case of $Pa\bar{3}$, the reflection conditions differ for the two twin components. [This is because the holohedry of $Pa\bar{3}$ is $m\bar{3}m$ whereas the Laue class of the Euclidean normalizer $Ia\bar{3}$ of $Pa\bar{3}$ is $m\bar{3}$; *cf.* *IT* A (1987, Part 15).] As a consequence, the reflection conditions for such a twinned crystal differ from all conditions that may be observed for single crystals (hkl cyclically permutable: $0kl$ only with $k = 2n$ *or* $l = 2n$; $00l$ only with $l = 2n$) and, therefore, the true symmetry can be identified without uncertainty.

In Table 1.3.4.2, all simulated Laue classes (column 1) are listed that may be observed for twins by merohedry of type 2. Column 2 shows the corresponding extinction symbols. The symbols of the simulated 'possible space groups' that follow from *IT* A (1983, Part 3) are gathered in column 3. The last column displays the symbols of those space groups which may be the true symmetry groups for twins by merohedry showing such diffraction patterns.

1.3.5. Calculation of the twin element

If the twin element cannot be recognized by direct macroscopic or microscopic inspection, it may be calculated as described below. Given are two analogous bases $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ and $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$ referring to the two twin components. If possible, both basis systems should be chosen with the same handedness. If no such bases exist, the twin is a reflection twin and one of the bases has to be replaced by its centrosymmetrical one, *e.g.* $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$ by $-\mathbf{a}'$, $-\mathbf{b}'$, $-\mathbf{c}'$. The relation between the two bases is described by

$$\begin{aligned}\mathbf{a}' &= e_{11}\mathbf{a} + e_{12}\mathbf{b} + e_{13}\mathbf{c},\\ \mathbf{b}' &= e_{21}\mathbf{a} + e_{22}\mathbf{b} + e_{23}\mathbf{c},\\ \mathbf{c}' &= e_{31}\mathbf{a} + e_{32}\mathbf{b} + e_{33}\mathbf{c}.\end{aligned}$$

The coefficients e_{ij} have to be obtained by measurement.

Basis $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ may be mapped onto $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$ by a pure rotation that brings $\mathbf{a}$ to $\mathbf{a}'$, $\mathbf{b}$ to $\mathbf{b}'$, and $\mathbf{c}$ to $\mathbf{c}'$. To derive the direction of the rotation axis, calculate the three vectors

$$\mathbf{a}_1 = \mathbf{a} + \mathbf{a}', \quad \mathbf{b}_1 = \mathbf{b} + \mathbf{b}', \quad \mathbf{c}_1 = \mathbf{c} + \mathbf{c}'.$$

$\mathbf{a}_1$, $\mathbf{b}_1$, $\mathbf{c}_1$ bisect the angles $\sigma_a = \mathbf{a} \wedge \mathbf{a}'$, $\sigma_b = \mathbf{b} \wedge \mathbf{b}'$, and $\sigma_c = \mathbf{c} \wedge \mathbf{c}'$, respectively. Calculate three further vectors of arbitrary length $\mathbf{a}_2$, $\mathbf{b}_2$, $\mathbf{c}_2$ which are perpendicular to the planes defined by $\mathbf{a}$ and $\mathbf{a}'$, $\mathbf{b}$ and $\mathbf{b}'$, and $\mathbf{c}$ and $\mathbf{c}'$, respectively, from the scalar products

$$\begin{aligned}\mathbf{a}_2 \cdot \mathbf{a} &= \mathbf{a}_2 \cdot \mathbf{a}' = 0,\\ \mathbf{b}_2 \cdot \mathbf{b} &= \mathbf{b}_2 \cdot \mathbf{b}' = 0,\\ \mathbf{c}_2 \cdot \mathbf{c} &= \mathbf{c}_2 \cdot \mathbf{c}' = 0.\end{aligned}$$

The plane defined by $\mathbf{a}_1$ and $\mathbf{a}_2$ is perpendicular to the plane defined by $\mathbf{a}$ and $\mathbf{a}'$ and bisects the angle $\mathbf{a} \wedge \mathbf{a}'$. Analogous planes refer to $\mathbf{b}_1$ and $\mathbf{b}_2$, and $\mathbf{c}_1$ and $\mathbf{c}_2$. Vectors $\mathbf{r}_a$, $\mathbf{r}_b$, and $\mathbf{r}_c$ lying within one of these planes may be described as linear combinations of $\mathbf{a}_1$ and $\mathbf{a}_2$, $\mathbf{b}_1$and $\mathbf{b}_2$, or $\mathbf{c}_1$ and $\mathbf{c}_2$, respectively:

$$\begin{aligned}\mathbf{r}_a &= \lambda_a\mathbf{a}_1 + \mu_a\mathbf{a}_2,\\ \mathbf{r}_b &= \lambda_b\mathbf{b}_1 + \mu_b\mathbf{b}_2,\\ \mathbf{r}_c &= \lambda_c\mathbf{c}_1 + \mu_c\mathbf{c}_2.\end{aligned}$$

The common intersection line of these three planes is parallel to the twin axis. It may be calculated by solving any of the three equations

$$\mathbf{r}_a = \mathbf{r}_b, \quad \mathbf{r}_a = \mathbf{r}_c, \quad \text{or} \quad \mathbf{r}_b = \mathbf{r}_c.$$

$\mathbf{r}_a = \mathbf{r}_b$: choose λ_a arbitrarily equal to 1.

$$\mathbf{a}_1 + \mu_a\mathbf{a}_2 = \lambda_b\mathbf{b}_1 + \mu_b\mathbf{b}_2.$$

Solve the inhomogeneous system of three equations that corresponds to this vector equation for the three variables μ_a, λ_b, and μ_b. Calculate the vector $\mathbf{r} = \mathbf{a}_1 + \mu_a\mathbf{a}_2$. Its components with respect to $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ describe the direction of the twin axis.

The angle τ of the twin rotation may then be calculated by

$$\sin\tfrac{1}{2}\tau = \frac{\sin\frac{1}{2}\sigma_a}{\sin\delta_a} = \frac{\sin\frac{1}{2}\sigma_b}{\sin\delta_b} = \frac{\sin\frac{1}{2}\sigma_c}{\sin\delta_c}$$

with $\delta_a = \mathbf{r} \wedge \mathbf{a}$, $\delta_b = \mathbf{r} \wedge \mathbf{b}$, $\delta_c = \mathbf{r} \wedge \mathbf{c}$.

If the basis $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ is orthogonal, τ may be obtained from

$$\cos\tau = \tfrac{1}{2}(\cos\sigma_a + \cos\sigma_b + \cos\sigma_c - 1).$$

If the coefficients of $\mathbf{r}$ are rational and τ equals 180°, then $\mathbf{r}$ describes the direction either of the twofold twin axis or of the normal of the twin plane. If $\mathbf{r}$ is rational and τ equals 60, 90 or 120°, $\mathbf{r}$ is parallel to the twin axis. If $\mathbf{r}$ is irrational, but τ equals 180° and there exists, in addition, a net plane perpendicular to $\mathbf{r}$, this net plane describes the twin plane.

If none of these conditions is fulfilled, one has to repeat the calculations with a differently chosen basis system for one of the twin components. The number of possibilities for this choice depends on the lattice symmetry. The following list gives all equivalent basis systems for all descriptions of Bravais lattices used in *IT* A (1983):

aP: $\mathbf{a}, \mathbf{b}, \mathbf{c}$;

mP, *mS* (unique axis **b**): $\mathbf{a}, \mathbf{b}, \mathbf{c}$; $-\mathbf{a}, \mathbf{b}, -\mathbf{c}$;

mP, *mS* (unique axis **c**): $\mathbf{a}, \mathbf{b}, \mathbf{c}$; $-\mathbf{a}, -\mathbf{b}, \mathbf{c}$;

oP, *oS*, *oI*, *oF*: $\mathbf{a}, \mathbf{b}, \mathbf{c}$; $-\mathbf{a}, -\mathbf{b}, \mathbf{c}$; $-\mathbf{a}, \mathbf{b}, -\mathbf{c}$; $\mathbf{a}, -\mathbf{b}, -\mathbf{c}$;

tP, *tI*: $\mathbf{a}, \mathbf{b}, \mathbf{c}$; $-\mathbf{a}, -\mathbf{b}, \mathbf{c}$; $-\mathbf{a}, \mathbf{b}, -\mathbf{c}$; $\mathbf{a}, -\mathbf{b}, -\mathbf{c}$; $\mathbf{b}, -\mathbf{a}, \mathbf{c}$; $-\mathbf{b}, \mathbf{a}, \mathbf{c}$; $\mathbf{b}, \mathbf{a}, -\mathbf{c}$; $-\mathbf{b}, -\mathbf{a}, -\mathbf{c}$;

hP: $\mathbf{a}, \mathbf{b}, \mathbf{c}$; $\mathbf{b}, -\mathbf{a}-\mathbf{b}, \mathbf{c}$; $-\mathbf{a}-\mathbf{b}, \mathbf{a}, \mathbf{c}$; $\mathbf{b}, \mathbf{a}, -\mathbf{c}$; $-\mathbf{a}-\mathbf{b}, \mathbf{b}, -\mathbf{c}$; $\mathbf{a}, -\mathbf{a}-\mathbf{b}, -\mathbf{c}$; $-\mathbf{a}, -\mathbf{b}, \mathbf{c}$; $-\mathbf{b}, \mathbf{a}+\mathbf{b}, \mathbf{c}$; $\mathbf{a}+\mathbf{b}, -\mathbf{a}, \mathbf{c}$; $-\mathbf{b}, -\mathbf{a}, -\mathbf{c}$; $\mathbf{a}+\mathbf{b}, -\mathbf{b}, -\mathbf{c}$; $-\mathbf{a}, \mathbf{a}+\mathbf{b}, -\mathbf{c}$;

hR (hexagonal description): $\mathbf{a}, \mathbf{b}, \mathbf{c}$; $\mathbf{b}, -\mathbf{a}-\mathbf{b}, \mathbf{c}$; $-\mathbf{a}-\mathbf{b}, \mathbf{a}, \mathbf{c}$; $\mathbf{b}, \mathbf{a}, -\mathbf{c}$; $-\mathbf{a}-\mathbf{b}, \mathbf{b}, -\mathbf{c}$; $\mathbf{a}, -\mathbf{a}-\mathbf{b}, -\mathbf{c}$;

hR (rhombohedral description): $\mathbf{a}, \mathbf{b}, \mathbf{c}$; $\mathbf{b}, \mathbf{c}, \mathbf{a}$; $\mathbf{c}, \mathbf{a}, \mathbf{b}$; $-\mathbf{b}, -\mathbf{a}, -\mathbf{c}$; $-\mathbf{a}, -\mathbf{c}, -\mathbf{b}$; $-\mathbf{c}, -\mathbf{b}, -\mathbf{a}$;

cP, *cI*, *cF*: $\mathbf{a}, \mathbf{b}, \mathbf{c}$; $\mathbf{b}, \mathbf{c}, \mathbf{a}$; $\mathbf{c}, \mathbf{a}, \mathbf{b}$; $-\mathbf{a}, -\mathbf{b}, \mathbf{c}$; $-\mathbf{b}, \mathbf{c}, -\mathbf{a}$; $\mathbf{c}, -\mathbf{a}, -\mathbf{b}$; $-\mathbf{a}, \mathbf{b}, -\mathbf{c}$; $\mathbf{b}, -\mathbf{c}, -\mathbf{a}$; $-\mathbf{c}, -\mathbf{a}, \mathbf{b}$; $\mathbf{a}, -\mathbf{b}, -\mathbf{c}$; $-\mathbf{b}, -\mathbf{c}, \mathbf{a}$; $-\mathbf{c}, \mathbf{a}, -\mathbf{b}$; $-\mathbf{b}, -\mathbf{a}, -\mathbf{c}$; $-\mathbf{a}, -\mathbf{c}, -\mathbf{b}$; $-\mathbf{c}, -\mathbf{b}, -\mathbf{a}$; $\mathbf{b}, \mathbf{a}, -\mathbf{c}$; $\mathbf{a}, -\mathbf{c}, \mathbf{b}$; $-\mathbf{c}, \mathbf{b}, \mathbf{a}$; $\mathbf{b}, -\mathbf{a}, \mathbf{c}$; $-\mathbf{a}, \mathbf{c}, \mathbf{b}$; $\mathbf{c}, \mathbf{b}, -\mathbf{a}$; $-\mathbf{b}, \mathbf{a}, \mathbf{c}$; $\mathbf{a}, \mathbf{c}, -\mathbf{b}$; $\mathbf{c}, -\mathbf{b}, \mathbf{a}$.