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(2) Orthorhombic lattice with $b = \sqrt{3}a$: [310] is perpendicular to (110).

(i) $P$ lattice (*cf.* Fig. 1.3.2.2):
$j = hu + kv + lw = 4$ even
$i = |j|/2 = 2$.

(ii) $C$ lattice (*cf.* also Fig. 1.3.2.2):
Because of the $C$ centring, [310] has to be replaced by $[\frac{3}{2}\frac{1}{2}0]$.
$j = hu' + kv' + lw' = 2$ even
$i = |j|/2 = 1$.

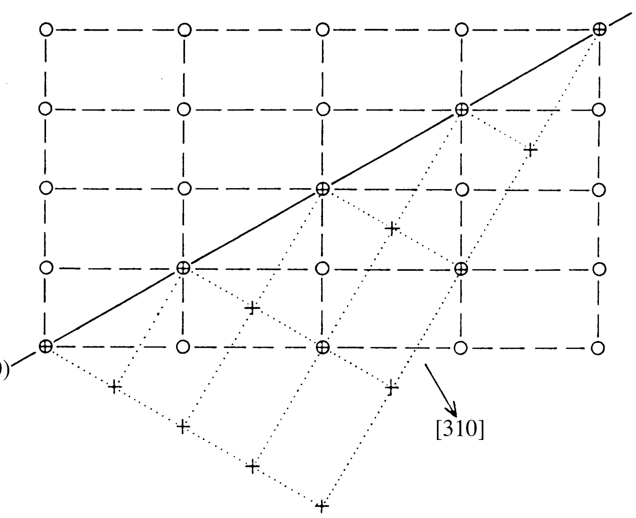


Fig. 1.3.2.2. Projection of the lattices of the twin components of an orthorhombic twinned crystal ($oP, b = \sqrt{3}a$) with twin index 2. The twin may be interpreted either as a rotation twin with twin axis [310] or as a reflection twin with twin plane (110). The figure shows, in addition, that twin index 1 results if the $oP$ lattice is replaced by an $oC$ lattice in this example (twinning by pseudomerohedry).

(3) Orthorhombic $C$ lattice with $b = 2a$: [210] is perpendicular to (120) (*cf.* Fig. 1.3.2.3).
As (120) refers to an 'extinct reflection' of a $C$ lattice, the triplet 240 has to be used in the calculation.
$j = h'u + k'v + l'w = 8$ even
$i = |j|/2 = 4$.

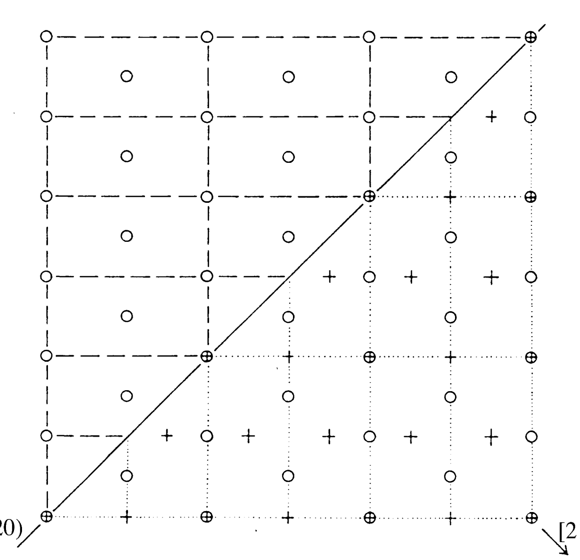


Fig. 1.3.2.3. Projection of the lattices of the twin components of an orthorhombic twinned crystal ($oC, b = 2a$) with twin index 4. The twin may be interpreted either as a rotation twin with twin axis [210] or as a reflection twin with twin plane (120).

(4) Rhombohedral lattice in hexagonal description with $c = \frac{1}{2}\sqrt{3}a$: $[\bar{1}1\bar{2}]$ is perpendicular to $(1\bar{1}1)$.
Because of the $R$ centring, $[\bar{1}1\bar{2}]$ has to be replaced by $[\bar{\frac{1}{3}}\frac{1}{3}\bar{\frac{2}{3}}]$.
As $(1\bar{1}1)$ refers to an 'extinct reflection' of an $R$ lattice, the triplet $1\bar{1}1$ has to be replaced by $3\bar{3}3$.
$j = h'u' + k'v' + l'w' = -4$ even
$i = |j|/2 = 2$.

### 1.3.3. Implication of twinning in reciprocal space

As shown above, the direct lattices of the components of any twin coincide in at least one row. The same is true for the corresponding reciprocal lattices. They coincide in all rows perpendicular to parallel net planes of the direct lattices.

For a reflection twin with twin plane ($hkl$), the reciprocal lattices of the twin components have only the lattice points with coefficients $nh$, $nk$, $nl$ in common.

For a rotation twin with twofold twin axis [$uvw$], the reciprocal lattices of the twin components coincide in all points of the plane perpendicular to [$uvw$], *i.e.* in all points with coefficients $h$, $k$, $l$ that fulfil the condition $hu + kv + lw = 0$.

For a rotation twin with irrational twin axis parallel to a net plane ($hkl$), only reciprocal-lattice points with coefficients $nh$, $nk$, $nl$ are common to both twin components.

As the entire direct lattices of the two twin components coincide for an inversion twin, the same must be true for their reciprocal lattices.

For a reflection or rotation twin with a twin lattice of index $i$, the corresponding reciprocal lattices, too, have a sublattice with index $i$ in common (*cf*. Fig. 1.3.2.1*b*). In analogy to direct space, the twin lattice in reciprocal space consists of each $i$th lattice plane parallel to the twin plane or perpendicular to the twin axis. If the twin index equals 1, the entire reciprocal lattices of the twin components coincide.

If for a reflection twin there exists only a lattice row [$uvw$] that is almost (but not exactly) perpendicular to the twin plane ($hkl$), then the lattices of the two twin components nearly coincide in a three-dimensional subset of lattice points. The corresponding misfit is described by the quantity $\omega$, the *twin obliquity*. It is the angle between the lattice row [$uvw$] and the direction perpendicular to the twin plane ($hkl$). In an analogous way, the twin obliquity $\omega$ is defined for a rotation twin. If ($hkl$) is a net plane almost (but not exactly) perpendicular to the twin axis [$uvw$], then $\omega$ is the angle between [$uvw$] and the direction perpendicular to ($hkl$).

### 1.3.4. Twinning by merohedry

A twin is called a *twin by merohedry* if its twin operation belongs to the point group of its vector lattice, *i.e.* to the corresponding holohedry. As each lattice is centrosymmetric, an inversion twin is necessarily a twin by merohedry. Only crystals from merohedral (*i.e.* non-holohedral) point groups may form twins by merohedry; 159 out of the 230 types of space groups belong to merohedral point groups.

For a twin by merohedry, the vector lattices of all twin components coincide in direct *and* in reciprocal space. The twin index is 1. The maximal number of differently oriented twin components equals the subgroup index $m$ of the point group of the crystal with respect to its holohedry.

Table 1.3.4.1 displays all possibilities for twinning by merohedry. For each holohedral point group (column 1), the types of Bravais lattices (column 2) and the corresponding merohedral point groups (column 3) are listed. Column 4 gives the subgroup index $m$ of a merohedral point group in its



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Table 1.3.4.1. *Possible twin operations for twins by merohedry*

$m$ is the index of the point group in the corresponding holohedry; point groups allowing twins of type 2 are marked by an asterisk.

| Holohedry | Bravais lattice | Point group | $m$ | Possible twin operations |
|---|---|---|---|---|
| 1 | $aP$ | 1 | 2 | $\bar{1}$ |
| $2/m$ | $mP, mS$ | 2 | 2 | $\bar{1}$ |
| | | $m$ | 2 | $\bar{1}$ |
| $mmm$ | $oP, oS, oI, oF$ | 222 | 2 | $\bar{1}$ |
| | | $mm2$ | 2 | $\bar{1}$ |
| $4/mmm$ | $tP, tI$ | *4 | 4 | $\bar{1}$, $.m.$, $.2.$ |
| | | *$\bar{4}$ | 4 | $\bar{1}$, $.m.$, $.2.$ |
| | | *$4/m$ | 2 | $.m.$ |
| | | 422 | 2 | $\bar{1}$ |
| | | $4mm$ | 2 | $\bar{1}$ |
| | | $\bar{4}2m/\bar{4}m2$ | 2 | $\bar{1}$ |
| $\bar{3}m$ | $hR$ | *3 | 4 | $\bar{1}$, $.m$, $.2$ |
| | | *$\bar{3}$ | 2 | $.m$ |
| | | 32 | 2 | $\bar{1}$ |
| | | $3m$ | 2 | $\bar{1}$ |
| $6/mmm$ | $hP$ | *3 | 8 | $\bar{1}$, $.m.$, $.2.$, $m..$, $..m$, $2..$, $..2$ |
| | | *$\bar{3}$ | 4 | $.m.$, $m..$, $..m$ |
| | | *321/312 | 4 | $\bar{1}$, $m..$, $..2/.2.$ |
| | | *$3m1/31m$ | 4 | $\bar{1}$, $m..$, $..m/.m.$ |
| | | *$\bar{3}m1/\bar{3}1m$ | 2 | $m..$ |
| | | *6 | 4 | $\bar{1}$, $.m.$, $.2.$ |
| | | *$\bar{6}$ | 4 | $\bar{1}$, $.m.$, $..m$ |
| | | *$6/m$ | 2 | $.m.$ |
| | | 622 | 2 | $\bar{1}$ |
| | | $6mm$ | 2 | $\bar{1}$ |
| | | $\bar{6}2m/\bar{6}m2$ | 2 | $\bar{1}$ |
| $m\bar{3}m$ | $cP, cI, cF$ | *23 | 4 | $\bar{1}$, $..m$, $..2$ |
| | | *$m\bar{3}$ | 2 | $..m$ |
| | | 432 | 2 | $\bar{1}$ |
| | | $\bar{4}3m$ | 2 | $\bar{1}$ |

holohedry. Column 5 shows $m-1$ possible twin operations referring to the different twin components. These twin operations are not uniquely defined (except for point group 1), but may be chosen arbitrarily from the corresponding right coset of the crystal point group in its holohedry. It is always possible, however, to choose an inversion, a reflection, or a twofold rotation as twin operation.

A twin that is not a twin by merohedry as defined above but, because of metrical specialization, has a twin lattice with twin index 1 is called a *twin by pseudo-merohedry*.

Two kinds of twins by merohedry may be distinguished.

*Type* 1: The twin can be described as an inversion twin. Then, only two twin components exist and the twin operation belongs to the Laue class of the crystal. As a consequence, the reciprocal lattices of the twin components are superimposed so that coinciding lattice points refer to Bragg reflections with the same $|F|^2$ values as long as Friedel's law is valid. In that case, no differences with respect to symmetry, or to reflection conditions, or to relative intensities occur between two sets of Bragg intensities measured from a single crystal on the one hand and from a twin on the other hand (whether or not the twin components differ in their volumes). If anomalous scattering is observed *and* the twin components differ in size, the intensities of Bragg reflections are changed in comparison with the untwinned crystal but the symmetry of the diffraction pattern is unchanged. For equal volumes of the twin components, however, the diffraction pattern is centrosymmetric again. The occurrence of anomalous scattering does not produce additional difficulties for space-group determination. The change of the

Table 1.3.4.2. *Simulated Laue classes, extinction symbols, simulated 'possible space groups', and possible true space groups for crystals twinned by merohedry (type 2)*

| Twinned crystal | | | Single crystal |
|---|---|---|---|
| Simulated Laue class | Twin extinction symbol | Simulated 'possible space groups' | Possible true space groups |
| $4/mmm$ | $P---$ | $P422$, $P4mm$, $P\bar{4}2m$, $P\bar{4}m2$, $P4/mmm$ | $P4$, $P\bar{4}$, $P4/m$ |
| | $P4_2--$ | $P4_222$ | $P4_2$, $P4_2/m$ |
| | $P4_1--$ | $P4_122$, $P4_322$ | $P4_1$, $P4_3$ |
| | $Pn--$ | $P4/nmm$ | $P4/n$ |
| | $P4_2/n--$ | – | $P4_2/n$ |
| | $I---$ | $I422$, $I4mm$, $I\bar{4}2m$, $I\bar{4}m2$, $I4/mmm$ | $I4$, $I\bar{4}$, $I4/m$ |
| | $I4_1--$ | $I4_122$ | $I4_1$ |
| | $I4_1/a--$ | – | $I4_1/a$ |
| $\bar{3}m1$ | $P---$ | $P321$, $P3m1$, $P\bar{3}m1$ | $P3$, $P\bar{3}$ |
| | $P3_1--$ | $P3_121$, $P3_221$ | $P3_1$, $P3_2$ |
| $\bar{3}1m$ | $P---$ | $P312$, $P31m$, $P\bar{3}1m$ | $P3$, $P\bar{3}$ |
| | $P3_1--$ | $P3_112$, $P3_212$ | $P3_1$, $P3_2$ |
| $\bar{3}m$ | $R--$ | $R32$, $R3m$, $R\bar{3}m$ | $R3$, $R\bar{3}$ |
| $6/m$ | $P---$ | $P6$, $P\bar{6}$, $P6/m$ | $P3$, $P\bar{3}$ |
| | $P6_2--$ | $P6_2$, $P6_4$ | $P3_1$, $P3_2$ |
| $6/mmm$ | $P---$ | $P622$, $P6mm$, $P\bar{6}m2$, $P\bar{6}2m$, $P6/mmm$ | $P3$, $P\bar{3}$, $P321$, $P312$, $P3m1$, $P31m$, $P\bar{3}m1$, $P\bar{3}1m$, $P6$, $P\bar{6}$, $P6/m$ |
| | $P6_3--$ | $P6_322$ | $P6_3$, $P6_3/m$ |
| | $P6_2--$ | $P6_222$, $P6_422$ | $P3_1$, $P3_2$, $P3_121$, $P3_221$, $P3_112$, $P3_212$, $P6_2$, $P6_4$ |
| | $P6_1--$ | $P6_122$, $P6_522$ | $P6_1$, $P6_5$ |
| | $P--c$ | $P6_3mc$, $P\bar{6}2c$, $P6_3/mmc$ | $P31c$, $P\bar{3}1c$ |
| | $P-c-$ | $P6_3cm$, $P\bar{6}c2$, $P6_3/mcm$ | $P3c1$, $P\bar{3}c1$ |
| $m\bar{3}m$ | $P---$ | $P432$, $P\bar{4}3m$, $Pm\bar{3}m$ | $P23$, $Pm\bar{3}$ |
| | $P4_2--$ | $P4_232$ | $P2_13$ |
| | $Pn--$ | $Pn\bar{3}m$ | $Pn\bar{3}$ |
| | $I---$ | $I432$, $I\bar{4}3m$, $Im\bar{3}m$ | $I23$, $I2_13$, $Im\bar{3}$ |
| | $Ia--$ | – | $Ia\bar{3}$ |
| | $F---$ | $F432$, $F\bar{4}3m$, $Fm\bar{3}m$ | $F23$, $Fm\bar{3}$ |
| | $Fd--$ | $Fd\bar{3}m$ | $Fd\bar{3}$ |
| | $P2_1/a, b--$ | – | $Pa\bar{3}$ |

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 **a**, **b**, **c** and **a**′, **b**′, **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.* **a**′, **b**′, **c**′ by −**a**′, −**b**′, −**c**′. The relation between the two bases is described by

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

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

Basis **a**, **b**, **c** may be mapped onto **a**′, **b**′, **c**′ by a pure rotation that brings **a** to **a**′, **b** to **b**′, and **c** to **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 **a** and **a**′, **b** and **b**′, and **c** and **c**′, respectively, from the scalar products

$$\mathbf{a}_2 \cdot \mathbf{a} = \mathbf{a}_2 \cdot \mathbf{a}' = 0,$$
$$\mathbf{b}_2 \cdot \mathbf{b} = \mathbf{b}_2 \cdot \mathbf{b}' = 0,$$
$$\mathbf{c}_2 \cdot \mathbf{c} = \mathbf{c}_2 \cdot \mathbf{c}' = 0.$$

The plane defined by $\mathbf{a}_1$ and $\mathbf{a}_2$ is perpendicular to the plane defined by **a** and **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:

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

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 $\lambda_a$ 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 $\mu_a$, $\lambda_b$, and $\mu_b$. Calculate the vector $\mathbf{r} = \mathbf{a}_1 + \mu_a\mathbf{a}_2$. Its components with respect to **a**, **b**, **c** describe the direction of the twin axis.

The angle $\tau$ 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 **a**, **b**, **c** is orthogonal, $\tau$ may be obtained from

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

If the coefficients of **r** are rational and $\tau$ equals 180°, then **r** describes the direction either of the twofold twin axis or of the normal of the twin plane. If **r** is rational and $\tau$ equals 60, 90 or 120°, **r** is parallel to the twin axis. If **r** is irrational, but $\tau$ equals 180° and there exists, in addition, a net plane perpendicular to **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*: **a**, **b**, **c**;

*mP*, *mS* (unique axis **b**): **a**, **b**, **c**; −**a**, **b**, −**c**;

*mP*, *mS* (unique axis **c**): **a**, **b**, **c**; −**a**, −**b**, **c**;

*oP*, *oS*, *oI*, *oF*: **a**, **b**, **c**; −**a**, −**b**, **c**; −**a**, **b**, −**c**; **a**, −**b**, −**c**;

*tP*, *tI*: **a**, **b**, **c**; −**a**, −**b**, **c**; −**a**, **b**, −**c**; **a**, −**b**, −**c**;
**b**, −**a**, **c**; −**b**, **a**, **c**; **b**, **a**, −**c**; −**b**, −**a**, −**c**;

*hP*: **a**, **b**, **c**; **b**, −**a** − **b**, **c**; −**a** − **b**, **a**, **c**; **b**, **a**, −**c**;
−**a** − **b**, **b**, −**c**; **a**, −**a** − **b**, −**c**; −**a**, −**b**, **c**; −**b**, **a** + **b**, **c**;
**a** + **b**, −**a**, **c**; −**b**, −**a**, −**c**; **a** + **b**, −**b**, −**c**; −**a**, **a** + **b**, −**c**;

*hR* (hexagonal description): **a**, **b**, **c**; **b**, −**a** − **b**, **c**;
−**a** − **b**, **a**, **c**; **b**, **a**, −**c**; −**a** − **b**, **b**, −**c**; **a**, −**a** − **b**, −**c**;

*hR* (rhombohedral description): **a**, **b**, **c**; **b**, **c**, **a**; **c**, **a**, **b**;
−**b**, −**a**, −**c**; −**a**, −**c**, −**b**; −**c**, −**b**, −**a**;

*cP*, *cI*, *cF*: **a**, **b**, **c**; **b**, **c**, **a**; **c**, **a**, **b**; −**a**, −**b**, **c**;
−**b**, **c**, −**a**; **c**, −**a**, −**b**; −**a**, **b**, −**c**; **b**, −**c**, −**a**;
−**c**, −**a**, **b**; **a**, −**b**, −**c**; −**b**, −**c**, **a**; −**c**, **a**, −**b**;
−**b**, −**a**, −**c**; −**a**, −**c**, −**b**; −**c**, −**b**, −**a**; **b**, **a**, −**c**;
**a**, −**c**, **b**; −**c**, **b**, **a**; **b**, −**a**, **c**; −**a**, **c**, **b**; **c**, **b**, −**a**;
−**b**, **a**, **c**; **a**, **c**, −**b**; **c**, −**b**, **a**.



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