Z. Kristallogr. **219** (2004) 57–71



# Twin point groups and the polychromatic symmetry of twins

Massimo Nespolo*

Université Henri Poincaré Nancy 1, Laboratoire de Cristallographie et de Modélisation des Matériaux Minéraux et Biologiques (LCM³B), UMR - CNRS 7036, Faculté de Sciences et Techniques, Boulevard des Aiguillettes, BP 239, F-54506 Vanduvre-lès-Nancy cedex, France

Received July 7, 2003; accepted October 20, 2003

*Colour symmetry / Geminography / Merohedry / Polychromatic point groups / Symmetry of twins / Twin point groups*

**Abstract.** A new classification in terms of the number of independent twin elements is introduced and exploited to analyze the symmetry of multiple twins. The dichromatic point group description of twins is revised showing that, contrary to what stated in the previous literature, all the 58 dichromatic point groups represent the possible symmetry of some twins. This approach is extended in terms of polychromatic point groups and applied to some examples from the recent literature.

## Introduction

J. D. H. Donnay introduced the term ***geminography*** to label the branch of crystallography which deals with twinning (Nespolo and Ferraris, 2003). In this way, he wanted to emphasize that twinned crystals are themselves a specific object of investigation, which needs a specific background knowledge. Nowadays, instead, twins are rather considered an obstacle to the routine structural work, and their description is often imprecise or unorthodox (see the examples given in Nespolo and Ferraris, 2004).

As a whole, a twin does not possess a homogeneous crystal structure: it is in fact a *heterogeneous edifice* built by two or more homogeneous crystals of the same crystallographic and chemical species (the "individuals") in different, non-equivalent orientations, related by point group operation(s) [the twin operation(s)] (Friedel, 1904). The symmetry of a twin is characterized by three components: 1. the symmetry of the individual, as expressed by its vector point group; 2. the symmetry of the lattice of the individual, $\mathbf{L}_\mathrm{I}$; 3. the symmetry of the twin lattice, $\mathbf{L}_\mathrm{T}$. The twin lattice $\mathbf{L}_\mathrm{T}$ consists of those nodes of $\mathbf{L}_\mathrm{I}$ which overlap (exactly or approximately) in the orientations of the twin individuals. Two parameters characterize $\mathbf{L}_\mathrm{T}$ with respect to $\mathbf{L}_\mathrm{I}$: the *twin index* $n_\mathrm{T}$ [inverse of the fraction of nodes of $\mathbf{L}_\mathrm{I}$ restored by the twin operation(s)], and the *twin obliquity* $\omega$ (the angle measuring the divergence of corresponding lattice rows or planes in $\mathbf{L}_\mathrm{T}$ and in $\mathbf{L}_\mathrm{I}$). Accordingly, twinning is classified in the following categories (Donnay and Donnay, 1974; Nespolo and Ferraris, 2000, 2004):

1. TLS (Twin Lattice Symmetry), $\omega = 0$;
1.1. *twinning by syngonic merohedry*, $n_\mathrm{T} = 1$: $\mathbf{L}_\mathrm{T}$ coincides with $\mathbf{L}_\mathrm{I}$, the point group of the individual is merohedral, the twin operation is a symmetry operation for the lattice but not for the individual;
1.2. *twinning by metric merohedry*, $n_\mathrm{T} = 1$: $\mathbf{L}_\mathrm{T}$ coincides again with $\mathbf{L}_\mathrm{I}$, but it has a specialized metric whose point symmetry is higher than the holohedry of the crystal, and the twin operation belongs to this higher lattice metric symmetry;
1.3. *twinning by reticular polyholohedry*, $n_\mathrm{T} > 1$: $\mathbf{L}_\mathrm{T}$ is a sublattice of $\mathbf{L}_\mathrm{I}$ (lower translational symmetry) with the same point symmetry, and the twin operation belongs to the symmetry of $\mathbf{L}_\mathrm{T}$ but not to the symmetry of $\mathbf{L}_\mathrm{I}$;
1.4. *twinning by reticular merohedry*, $n_\mathrm{T} > 1$: $\mathbf{L}_\mathrm{T}$ is a sublattice of $\mathbf{L}_\mathrm{I}$ (lower translational symmetry) with different point symmetry, and the twin operation belongs to the symmetry of $\mathbf{L}_\mathrm{T}$ but not to the symmetry of $\mathbf{L}_\mathrm{I}$.
2. TLQS (Twin Lattice Quasi Symmetry), $\omega > 0$;
2.1. *twinning by pseudo-merohedry*, $n_\mathrm{T} = 1$: for $\omega = 0$ it reduces to twinning by syngonic merohedry;
2.2. *twinning by reticular pseudo-polyholohedry*, $n_\mathrm{T} > 1$: for $\omega = 0$ it reduces to twinning by reticular polyholohedry;
2.3. *twinning by reticular pseudo-merohedry*, $n_\mathrm{T} > 1$: for $\omega = 0$ it reduces to twinning by reticular merohedry; for $n_\mathrm{T} = 1$ and $\omega = 0$ it reduces instead to twinning by metric merohedry.

## Twin point groups

The concept of "twin point groups" or "symmetry groups of twins" has already been used in the past by some authors, who however often introduced unjustified limitations, taking for a rule what was just a relative frequency of occurrence. For example, the existence of twin axes of order higher than 2 was repeatedly denied (e.g. Hartmann, 1956), although already Friedel (1904, 1926) had shown examples of their occurrences.

* e-mail: massimo.nespolo@lcm3b.uhp-nancy.fr

Takano (1972, 1973) introduced a classification of twin point groups that expresses the morphological symmetry of the *geometrical polyhedron* corresponding to the twinned edifice, i.e. as if the individuals had always symmetry 1.

Curien and Le Corre (1958) applied Shubnikov's dichromatic groups (Le Corre, 1958) to the symmetry analysis of twins, but they assumed that the twin point group had to belong to the same crystal family of the individuals' point group. While this frequently is the case, the limitation in itself is unjustified and contradicted by several examples.

In the following, we present a general symmetry treatment of twins in terms of polychromatic point groups. For that purpose, we need first of all to introduce a few definitions.

## Multiplicity and degree of a twin

***Twin operation*** is a symmetry operation for the twinned edifice but not for the individuals: it relates different individuals in the twin. ***Twin law*** is the set of all twin operations that transform two twinned individuals into each other. ***Twin element*** is the geometric elements about which the twin operation is performed (Hahn and Klapper, 2003). A mirror or a centre is either a symmetry element or a twin element. An axis [*uvw*] can act both as twin element and as (non-trivial) symmetry element if the operation performed about it is of order four or six, the two-fold or the three-fold components representing the symmetry operations.

We call ***twin multiplicity*** the number of individuals in a twin; and ***twin degree*** the number of independent twin elements: first-degree twins and higher-degree twins are twins in which only one or more than one *independent* twin elements exist, respectively. Higher-degree twins have been called "twins of twins" by Henke (2003).

Let $O^T_j$ be the order of the j-th twin element, and $O^S_j$ the order of the same element as symmetry element for the individual: $O^T_j \geq O^S_j$ depending on whether a component of the same element acts as symmetry element for the individual or not. If $m$ is the twin multiplicity, and $d$ is the twin degree, twins can be classified in the following types:

1 ***twofold twins:*** only twin elements of order 2 exist. These are subdivided in:
  - 1.1 ***first-degree twofold twins*** (*binary twins*): $d = 1$, $O^T_1/O^S_1 = 2$, $m = 2$.
  - 1.2 ***higher-degree twofold twins:*** $d > 1$, $O^T_j/O^S_j = 2\ \forall$ j, $m = 2d$.

2 ***manifold twins:*** at least one twin element has order higher than 2. They are subdivided in:
  - 2.1 ***first-degree manifold twins:*** the (only) twin element has order higher than 2 ($d = 1$, $m = O^T_1/O^S_1 > 2$)
  - 2.2 ***higher-degree manifold twins:*** at least one twin element has order higher than 2 ($d > 1$, $O^T_j/O^S_j > 2,\ m > 2$)

The twin multiplicity obeys the following relation:

$$m \leq m' = \prod_{i=1}^{d} \frac{O_j^T}{O_j^S} \tag{1}$$

For twofold twins, $m = m'$ always holds: in fact, a twofold (independent) twin element necessarily doubles the number of individuals. However, for manifold twins $m < m'$ may hold, when the number of individuals related by one or more twin elements is lower than the order of that twin element. As we will see, when $m < m'$, one or more twin operations no longer correspond to a symmetry operation, but rather to a *partial operation*, as defined by Sadanaga et al. (1980).

## The polychromatic group notation for twins

Curien and Le Corre (1958) have applied the dichromatic point group notation developed by Shubnikov to the description of the twin laws. Their treatment is however affected by some limitations. First of all, as noted by Shafranovkii and Pis'mennyi (1961) and stated also by Hahn and Klapper (2003), the dichromatic notation can describe only twofold twins, whereas manifold twins require a polychromatic description.

The second limitation in Curien and Le Corre (1958) comes from the fact that those authors assumed that the symmetry of the individual and that of the twin must belong to the same crystal family. Under this hypothesis the order ratio between the twin point group and its maximal subgroup (the individual monochromatic point group) is always two: this permits a description in terms of dichromatic groups. However, only 26 of the 32 crystallographic point groups are taken into account: the 25 merohedries and the rhombohedral holohedry (hemihedry of the hexagonal holohedry). For each of these 26 monochromatic point groups Curien and Le Corre (1958) derived the possible dichromatic point groups by taking the minimal supergroups in the same crystal family, obtaining 43 of the 58 dichromatic point groups. The remaining 15 were considered impossible as twin point groups, because they belong to a crystal family different from that of the monochromatic group (see Table III therein).

The limitation imposed on the crystal family is not justified and has lead to exclude not only twinning by metric merohedry, but also most cases of twinning by reticular merohedry. In the latter case, the orientation of the cell of $\mathbf{L}_T$ with respect to that of $\mathbf{L}_I$ is fixed only for the *hP* supercell of cubic and rhombohedral crystals [cf. Table II in Curien and Le Corre (1958)]. In all others cases, the orientation depends on the axial ratio (uniaxial crystals) and on the interaxial angle (biaxial crystals).

Moreover, the term *complete twin*, introduced by Curien and Donnay (1959) to indicate a twinned "edifice that comprises, in addition to an original crystal, as many twinned crystals as there are possible twin laws", becomes practically undefined once the limitation on the crystal family is removed. In fact, the only upper limits to "possible twin laws" are those imposed by the cubic and hexagonal holohedries. We give below a revised definition of "complete twin".

Let $\mathcal{K}^{(p)}$ be the polychromatic twin point group ($p$ being the chromaticity, namely the number of individuals related by the twin operations), and $\mathcal{H}$ be the monochromatic (geometric or eigensymmetry) point group of the individual. If $\mathcal{K}^{(p)}$ represents a first-degree twin, then $\mathcal{K}^{(p)}$ and $\mathcal{H}$ are in relation of minimal supergroup/maximal subgroup. If $\mathcal{K}^{(p)}$ represents instead a higher-degree twin, we can break down $\mathcal{K}^{(p)}$ in a series of $n$ maximal subgroups, $\mathcal{K}^{(p)} \subset \mathcal{K}_1^{(p_1)} \subset \mathcal{K}_2^{(p_2)} \cdots \subset \mathcal{H}$. Therefore, the twin point groups can be obtained by considering the pairs of crystallographic point groups in relation of minimal supergroup, for which the order ratio is 2, 3 or 4 (see Fig. 10.1.3.2 in Hahn and Klapper, 2002).

## Classification of polychromatic point groups and application to first-degree twins

The detailed derivation of polychromatic groups can be found in Shubnikov and Koptsik (1974); Vainsthein (1996) gave a brief summary; Wittke and Garrido (1959) and Van der Warden and Burckhardt, (1961) derived the noninvariant extensions of monochromatic point groups. Here we briefly summarize the results needed for the analysis of the symmetry of twins.

The number $k$ of chromaticities $p_k$ compatible with the crystallographic symmetry is 10 and corresponds to the orders of the crystallographic point groups: $p_k = 1, 2, 3, 4, 6, 8, 12, 16, 24, 48$. $p_1 = 1$ corresponds to the trivial case of monochromatic symmetry.

The direct product ($\mathcal{H}$, $1^{(p)}$) of the monochromatic point group $\mathcal{H}$ with the colour identification group $1^{(p)}$, consisting of all possible permutations of $p$ colours, produces 320 ***neutral*** point groups (i.e. point groups in which each geometric operation is associated with all the $p$ colours). Of these, 32 are the monochromatic point groups ($\mathcal{H}$, $1^{(1)}$), 32 are grey point groups ($\mathcal{H}$, $1^{(2)}$) and 256 are neutral polychromatic point groups ($\mathcal{H}$, $1^{(p>2)}$).

True (non-neutral) polychromatic point groups $\mathcal{K}^{(p)}$ isomorphic with the crystallographic monochromatic point groups $\mathcal{H}$ are obtained as extensions of the subgroups of $\mathcal{H}$ of order $p$. Invariant extension gives 51 dichromatic point groups ("black and white" groups, Shubnikov groups, $\mathcal{K}^{(2)}$), and 81 polychromatic point groups (Koptisk groups, $\mathcal{K}^{(p>2)}$)[1].

Other 73 true polychromatic point groups are obtained as noninvariant extensions and are termed Van der Waerden-Burckhardt groups, $\mathcal{K}_{WB}{}^{(p>2)}$ (the Wittke-Garrido groups, $\mathcal{K}_{WG}{}^{(p>2)}$, are isomorphous to them).

$\mathcal{K}^{(p)}$ and $\mathcal{K}_{WB}{}^{(p)}$ differ in the fact that all the elements in $\mathcal{K}^{(p)}$ are either *achromatic* (do not modify any colour) or *totally chromatic* (modify all the colours), whereas in $\mathcal{K}_{WB}{}^{(p>2)}$ some of the elements are *partially chromatic*: they preserve some of the colours on which they act, and exchange the others.

Summing up, there are 212 crystallographic truly polychromatic point groups (in three dimensions): of these, 58 are dichromatic ($\mathcal{K}^{(2)}$), 81 are polychromatic invariant extensions of $\mathcal{H}$ ($\mathcal{K}^{(p>2)}$), and 73 polychromatic noninvariant extensions of $\mathcal{H}$ ($\mathcal{K}_{WB}{}^{(p>2)}$). We will see that these three types are needed to described the symmetry of twins. But first of all, the symbolism for the polychromatic groups has to be reviewed briefly. In the following subsections, symbols for first-degree twins are described. The groups describing higher-degree twins are given later.

### Dichromatic extension of crystallographic point groups (Shubnikov groups)

These twin point groups, $\mathcal{K}^{(2)}$, are minimal supergroups of order two of the monochromatic groups $\mathcal{H}$. $\mathcal{H}$ are thus normal (invariant) subgroups of $\mathcal{K}^{(2)}$ ($\mathcal{K}^{(2)} \triangleright \mathcal{H}$). Only binary (first-degree twofold) twins can be described by $\mathcal{K}^{(2)}$ groups. If the original individual is considered "white", the one generated by a twin operation is considered "black" and the twin operation is marked with a prime ($'$). The symmetry of a binary twin point group corresponds thus to one of the 58 dichromatic point groups, where the symmetry elements are unprimed and the twin elements are primed. This is the symmetry of the vector set of face normals of the twin, exactly as the monochromatic point group expresses the symmetry of the vector set of face normals of the individual. For example, $42'2'$ indicates a twin by syngonic merohedry where the crystal point symmetry is 4 and the twin elements are the twofold axes along $\langle 100\rangle$ and $\langle 110\rangle$, which, being not independent, receive a prime each. $42'2'$ is in fact obtained as semidirect product of 4 and $2' \perp 4$.

When a twin axis is parallel to a symmetry axis ($O^T{}_j > O^S{}_j > 1$), the prime indicates the twin component. For example, $4'$ indicates an axis of order 4 about which the operations of odd order are twin operations, and those of even order are symmetry operation for the individual: $4' \supset 2$. The group $4'$ is obtained as semidirect product of $\{1, 2\}$ and of the coset consisting of the identity and the operation $4'$, which forms a group by modulus $4'$ (mod2): this type of product is called *quasi-direct product* and written $2 \odot 4'$ (mod2) (Shubnikov and Koptsik, 1974).

In the case of $n/m$ ($n$ even), the symmetry element and the twin element do not coalesce in a single symbol, giving instead $n/m'$ or $n'/m$ (the twin centre does not need to be explicitly denoted by $\bar{1}'$, because it is implied in the twin symbol).

All the 58 dichromatic point groups are possible twin point groups: the 15 groups which were considered not representative of possible twins by Curien and Le Corre (1958) correspond to minimal supergroups of order 2 belonging to *different* crystal families (Table 1). For example, the new mineral kristiansenite reported by Ferraris et al. (2001) is twinned by metric merohedry according to $m'$, which is one of the 15 twin dichromatic point groups considered "impossible" by Curien and Le Corre (1958). The monochromatic point group of the individual is $\mathcal{H} = 1$.

### Polychromatic invariant extension of crystallographic point groups (Koptsik groups)

In case of metric merohedry and of reticular merohedry, the twin point group and the individual group belong to different crystal families. As a consequence, the chromati-

[1] Chapter 10 of Shubnikov and Koptsik (1974), where this derivation is presented, was entirely written by Koptsik (see the *Resumé* therein). For brevity, we call $\mathcal{K}^{(p>2)}$ groups ***Koptsik groups***, to differentiate them from the dichromatic groups $\mathcal{K}^{(2)}$ which are universally known as ***Shubnikov groups***.

city $p$ for first-degree twins, which coincides with the order ratio of minimal supergroups (maximal subgroups), increases up to four. Among the 81 Kopstik $\mathcal{K}^{(p>2)}$ groups, 7 trichromatic $\mathcal{K}^{(3)}$ groups correspond to the symmetry of possible first-degree twins (Table 1) whose monochromatic groups $\mathcal{H}$ (*normal* maximal subgroups) belong to a different crystal family.

The symbol of a Koptsik group is based on the full Hermann-Mauguin symbol; to each chromatic element (twin element) a chromatic index $p_i$ is attached ($p_i = 2$ in Shubnikov groups is replaced by the prime $'$); finally, with the trivial exception of monosymbolic groups, the whole symbol is included in parenthesis and a chromatic index $p$ for the whole group is given. This corresponds to the ratio of the orders of $\mathcal{K}^{(p)}$ and $\mathcal{H}$, and for first-degree twins coincides with the chromatic index of the twin element ($p = p_1$).

**Examples.** Let us consider a crystal whose point group is 2, but having a hexagonal lattice or sublattice with 6 // 2. The six-fold axis is at the same time twin axis and symmetry axis: about it four twin operations ($6^1$, $6^3$, $6^4$ and $6^5$) and two symmetry operations ($6^3 = 2$ and $6^6 = 1$) are performed. The polychromatic symbol is $6^{(3)}$. 6 is the geometric symmetry operation for $\mathbf{L}_T$, which is trichromatic: it exchanges three colours, *i.e.* it relates three individuals. The two-fold component is the monochromatic symmetry operation of the individual, unchanged.

An orthorhombic crystal with symmetry 222 but with a cubic lattice or sublattice may undergo twinning by metric merohedry or by reticular merohedry, the twin element being the threefold axis along $\langle 111 \rangle$. The resulting symmetry of the twin is $(23^{(3)})^{(3)}$, which is the semidirect product of 222 and $3^{(3)}$.

## Polychromatic noninvariant extension of crystallographic point groups (Van der Waerden-Burckhardt groups)

The Koptsik groups $\mathcal{K}^{(p)}$ are obtained as invariant extensions of the monochromatic point groups $\mathcal{H}$. The 73 $\mathcal{K}_{\mathrm{WB}}{}^{(p)}$ polychromatic point groups are instead noninvariant extensions of $\mathcal{H}$. In other words, $\mathcal{H}$ are maximal *normal* subgroups with respect to $\mathcal{K}^{(p)}$ and maximal *conjugate* subgroups with respect to $\mathcal{K}_{\mathrm{WB}}{}^{(p)}$: $\mathcal{K}^{(p)} \triangleright \mathcal{H}$, $\mathcal{K}_{\mathrm{WB}}{}^{(p)} \ntriangleright \mathcal{H}$. Among $\mathcal{K}_{\mathrm{WB}}{}^{(p)}$, 14 groups of chromaticity $p = 3$ and 4 correspond to first-degree twins (Table 1).

A distinguishing feature of the $\mathcal{K}_{\mathrm{WB}}{}^{(p)}$ groups is the presence of elements $n^{(p_1,p_2)}$ of *partial chromaticity*: $p_1$ is the chromaticity of the element (same as seen for the Koptsik groups), whereas $p_2$ is the number of colours unchanged by the operations performed about that element. For example, an individual with monochromatic point group $\mathcal{H} = 2$ undergoing twinning by metric or reticular merohedry where the twin element is an axis of order 3 normal to the twofold axis of the individual, results in a three-individual twin with trichromatic point group $\mathcal{K}_{\mathrm{WB}}{}^{(3)} = (3^{(3)}2^{(2,1)})^{(3)}$. The chromaticity of the groups is 3 (three individuals in the twin; three is also the ratio of the order of point groups 32 and 2) and coincides with the chromaticity of the three-fold axis, which permutes the three individuals: $1 \to 2,\ 2 \to 3,\ 3 \to 1$, without leaving fixed any of them. But the twofold symmetry axis of the individual becomes partially chromatic: the twofold ration about it is a symmetry operations for the individual to which the axis belongs, and at the same time it exchanges the two other individuals: $2^{(2,1)}$.

The symbols of the $\mathcal{K}_{\mathrm{WB}}{}^{(p)}$ groups were introduced by Shubnikov and Koptsik (1974) and include three parts, $\mathcal{K} \mid \mathcal{H}_1 \mid \mathcal{H}_2$, where $\mathcal{K}$ is the polychromatic group, $\mathcal{H}_1$ is the noninvariant subgroup, and $\mathcal{H}_2$ is the invariant subgroup obtained as intersection of conjugate subgroups, all expressed in the axial setting of $\mathcal{K}$. Harker (1976) gave a complete list of the 212 crystallographic polychromatic point groups, as well as the icosahedral polychromatic point groups, with a simplified and unified notation employing shortened (instead of full) Hermann-Mauguin symbols, without indication of the chromaticity, and using the axial setting proper to each of the $\mathcal{K}$, $\mathcal{H}_1$, and $\mathcal{H}_2$ groups.

As symbols of twin groups we can use simply the $\mathcal{K}_{\mathrm{WB}}{}^{(p)}$ portion of the symbol, provided that the full information about the chromaticity of the group and of the elements is retained. The derivation of $\mathcal{H}$ from a given $\mathcal{K}_{\mathrm{WB}}{}^{(p)}$ is exemplified after the introduction of the groups for higher-degree twins.

## Twinning by syngonic merohedry

Because $\mathbf{L}_T \equiv \mathbf{L}_I$, the twin point groups are obtained from the monochromatic point groups $\mathcal{H}$ by taking the minimal supergroups of the same crystal family. These are minimal supergroups of order 2 and the corresponding twin point groups are thus dichromatic groups, $\mathcal{K}^{(2)}$. Column 2 in Table 1 gives the results, which are the same already obtained by Curien and Le Corre (1958). For the trigonal groups, however, the necessary distinction on the basis of the *hR* or *hP* lattice has been introduced.

## Twinning by metric merohedry and by reticular merohedry

No limitation on the symmetry of a sublattice can be imposed *a priori*, and the 15 dichromatic point groups considered impossible as twin point groups by Curien and Le Corre (1958) actually *do* represent possible twins (column 3 in Table 1). In this case, the dichromatic symbol may be less immediate to read, because one has to take into account the difference in the equivalent directions in the two crystal families. For example, an individual with monochromatic point group *mm*2 may undergo twinning by reticular merohedry or by metric merohedry with dichromatic point group $\bar{4}'m2'$. Here, the twofold axis of *mm*2 becomes parallel to the $\bar{4}$ axis of the twin, the two mirrors (100) and (010) become equivalent, and two twofold equivalent twin axes $2'$ appear along $\langle 110 \rangle$, which are not independent twin elements and thus receive the same number of primes (namely one) as $\bar{4}'$.

For metric merohedry, because $\mathbf{L}_T \equiv \mathbf{L}_I$, the list of twin point groups is exhaustive. For reticular merohedry, instead, with the exception of the cubic groups discussed below, the list is necessarily limited to the twins in which all the symmetry elements of the monochromatic point group are retained in the twin point group. Other possible cases are those in which only a part of those elements is retained: they include, for example, twins with inclined axes. The twin point group $\mathcal{K}$ is a supergroup no longer of $\mathcal{H}$ but of the intersection group of the individuals: $\mathcal{K} \supset \mathcal{H}^* = \cap\mathcal{H}_i$ (Hahn and Klapper, 2003). $\mathbf{L}_T$ is obtained as a function of the metrics of $\mathbf{L}_I$ by applying the Coincidence-Site Lattice (CSL) theory (see, e.g., Grimmer, 2003).

### Twinning by reticular merohedry of cubic crystals

Cubic groups do not have minimal supergroups belonging to a different family. Twinning by reticular merohedry is thus restricted to the case in which only a part of the symmetry elements of the monochromatic point group are retained in the twin point group. Whereas in non-isotropic crystals an exhaustive list cannot be given because the symmetry and orientation of $\mathbf{L}_T$ with respect to $\mathbf{L}_I$ depends on the metrics of the lattices, in cubic crystals there is no degree of freedom in the metric and thus such an exhaustive list can be given.

As it was pointed out by Curien and Le Corre (1958), (binary) twins by reticular merohedry are obtained via the trigonal subgroups of $\mathcal{H}$. Let $\mathcal{J}$ be the trigonal maximal subgroup of $\mathcal{H}$, where $\mathcal{H}$ is cubic ($\mathcal{J}$ is conjugate subgroup of order 4 of $\mathcal{H}$). Let $\mathcal{K}^{(2)}{}_{\mathcal{H},\mathrm{i}}$ be the $i$-th cubic minimal supergroup of $\mathcal{H}$ and $\mathcal{K}^{(2)}{}_{\mathcal{J},\mathrm{i}}$ the $i$-th trigonal or hexagonal minimal supergroups of $\mathcal{J}$: $\mathcal{K}^{(2)}{}_{\mathcal{H},\mathrm{i}} \triangleright \mathcal{H}$, $\mathcal{K}^{(2)}{}_{\mathcal{J},\mathrm{i}} \triangleright \mathcal{J}$ Twins by reticular merohedry of cubic crystals correspond to those $\mathcal{K}^{(2)}{}_{\mathcal{J},\mathrm{i}}$ groups which are not subgroups of $\mathcal{K}^{(2)}{}_{\mathcal{H},\mathrm{i}}$. For example, the trigonal component of the monochromatic point group $\mathcal{H} = 23$ is $\mathcal{J} = 3$. Of the eight minimal supergroups of $\mathcal{J}$, $\mathcal{K}^{(2)}{}_{\mathcal{J},\mathrm{i}} = 2'3$ is isomorphous with the original monochromatic group $\mathcal{H}$ and does not represent a twin; $\mathcal{K}^{(2)}{}_{\mathcal{J},\mathrm{i}} = \bar{3}'$, $32'1$ and $3m'1$ are normal subgroups of $\mathcal{K}^{(2)}{}_{\mathcal{H},\mathrm{i}} = 2/m'\bar{3}'$, $4'32'$ and $\bar{4}'3m'$ respectively, the latter representing twins by syngonic merohedry; only the four groups $\mathcal{K}^{(2)}{}_{\mathcal{J},\mathrm{i}} = 312'$, $31m'$, $6'$ and $\bar{6}'$ finally correspond to twinning by reticular merohedry.

### Twinning by reticular polyholohedry

In case of reticular polyholohedry, $\mathbf{L}_T$ and $\mathbf{L}_I$ have the same point symmetry, but non-equivalent orientations. $\mathcal{H}$ and $\mathcal{K}$ both correspond to the same holohedral point group, but the different orientation of $\mathbf{L}_T$ and $\mathbf{L}_I$ transforms some of the symmetry elements of $\mathcal{H}$ in twin elements. Like in the case of twins by reticular merohedry of cubic crystals, the passage from $\mathcal{H}$ to $\mathcal{K}$ requires an intermediate step through a subgroup $\mathcal{J}$ of $\mathcal{H}$. This time however the relation is more straightforward: $\mathcal{J}$ contains the symmetry elements which are parallel in $\mathbf{L}_I$ and $\mathbf{L}_T$, and in $\mathcal{K}$ the chromatic elements are those belonging to $\mathcal{H}$ but not to $\mathcal{J}$

For example, a tetragonal crystal may undergo twinning by reticular polyholohedry when the planes {120}, which are not symmetry planes for $\mathbf{L}_I$, act as twin elements. The relative orientation of $\mathbf{L}_T$ and $\mathbf{L}_I$ is defined by $c_{\mathbf{LT}} \,//\, c_{\mathbf{LI}}$ and $\langle 100\rangle_{\mathbf{LT}} \,//\, \langle 120\rangle_{\mathbf{LI}}$ (twin index 5). Evidently, $\mathcal{H} = 4/mmm$, $\mathcal{J} = 4/m$, $\mathcal{K}^{(2)} = 4/mm'm'$. Here $\mathcal{J}$ is the intersection symmetry of the two individuals differently oriented.

### Symbols for higher-degree twins

As shown in Table 1, all the 58 Shubnikov groups, 7 (all trichromatic) of the 81 Koptsik groups, and 15 (10 trichromatic and 5 quadricromatic) of the 73 Van der Waerden-Burckhardt groups represent the symmetry of first-degree twins. The remaining 132 polychromatic groups (74 $\mathcal{K}^{(p)}$ and 58 $\mathcal{K}_{\mathrm{WB}}{}^{(p)}$) represent higher-degree twins. Of these, only the twofold twins can be described by a composed dichromatic group as introduced by Curien and Donnay (1959): however, the polychromatic notation is more explicit and makes easier to identify the symmetry of the individuals and the twin elements. For example, the four-individual merohedric[2] twin of a tetartohedral cubic crystal has composed dichromatic symbol $\frac{4'}{m'} \supset [\bar{4}'''][\supset 2]3\frac{2''}{m'''}\bar{1}'$, whereas the polychromatic symbol is simply $\left(\frac{4^{(2)}}{m^{(2)}}\bar{3}^{(2)}\frac{2^{(2)}}{m^{(2)}}\right)^{(4)}$. For manifold twins, the composed dichromatic notation is not suitable and the polychromatic notation has no alternatives.

In Tables 2 and 3 the symbols of the $\mathcal{K}^{(p)}$ and $\mathcal{K}_{\mathrm{WB}}{}^{(p)}$ groups are given, together with the $\mathcal{H}$ groups of which they are supergroups. A sequence of twin elements is also given, which follows, whenever possible, the sequence of generators of the corresponding symmorphic space-group types in the *International Tables for Crystallography*, volume A: intermediate polychromatic groups $\mathcal{K}^{(p)}{}_i$ and $\mathcal{K}_{\mathrm{WB}}{}^{(p)}{}_i$ are easily obtained by taking the direct, semi-direct of quasi-direct product of $\mathcal{K}^{(p)}{}_{i-k}$ and $\mathcal{K}_{\mathrm{WB}}{}^{(p)}{}_{i-k}$ with the group $\{1, t_k\}$, where $t_k$ is the operation corresponding to the $k$-th twin element.

The meaning of the $\mathcal{K}^{(p)}$ symbols in terms of higher-degree twin point groups is practically self-explanatory (Table 2), whereas that of $\mathcal{K}_{\mathrm{WB}}{}^{(p)}$ is slightly more complex (Table 3) and requires thus a brief explanation.

For both $\mathcal{K}^{(p)}$ and $\mathcal{K}_{\mathrm{WB}}{}^{(p)}$, the chromaticity $p$ of the group represents the number of individuals, and corresponds to the ratio of the orders of the twin point group, $\mathcal{K}^{(p)}$ or $\mathcal{K}_{\mathrm{WB}}{}^{(p)}$, and of the monochromatic group of the individual, $\mathcal{H}$. The chromaticity $p_i$ of each element gives the number of individuals related ("exchanged") by that element. Evidently, $p_i$ is a divisor of the order of the geometric element. However, in $\mathcal{K}_{\mathrm{WB}}{}^{(p)}$ some of the symmetry elements of the individual acquire a partial chromaticity: these elements do not modify the individual to which they belong. Therefore, the elements of a twin point group have to be interpreted as follows (for further details, see Shubnikov and Koptsik, 1974):

1 achromatic elements (without a chromatic index $p_i$): symmetry elements for the individual which do not act as twin elements;

[2] The term "merohedral twin", often appearing in the literature, is misleading. "Merohedral", in contrast to "holohedral", is an adjective identifying a crystal whose point group is a subgroup of the point group of its lattice (Friedel, 1926). A merohedral crystal may undergo twinning by merohedry, in which the twin operation belongs to the lattice of the individual; the corresponding adjective is "merohedric" (Nespolo and Ferraris, 2003).

**Table 1.** Polychromatic point groups for first-degree twins. In dichromatic groups, the chromatic elements are shown with a prime. In polychromatic groups, the chromaticity of each element and of the groups is shown as superscript in parenthesis. Van der Waerden-Burckhardt groups include elements partially chromatic, which act on a subset of individuals.

| $\mathcal{H}$ | $\mathcal{K}^{(p)}$ | | | |
|---|---|---|---|---|
| | Twinning by syngonic merohedry: Shubnikov groups $\mathcal{K}^{(2)}$ | Twinning by metric merohedry or by reticular merohedry | | |
| | | Shubnikov groups $\mathcal{K}^{(2)}$ | Koptsik groups $\mathcal{K}^{(p>2)}$ | Van der Waerden-Burckhardt groups $\mathcal{K}_{\mathrm{WB}}{}^{(p>2)}$ |
| $1$ | $\bar{1}'$ | $m'$, $2'$, | $3^{(3)}$ | – |
| $\bar{1}$ | – | $2'/m'$ | $\bar{3}^{(3)}$ | – |
| $2$ | $2/m'$ | $m'm'2$, $2'2'2$, $4'$, $\bar{4}'$ | $6^{(3)}$ | $(3^{(3)}2^{(2,1)})^{(3)}$ |
| $m$ | $2'/m$ | $m'm2'$ | $\bar{6}^{(3)}$ | $(3^{(3)}m^{(2,1)})^{(3)}$ |
| $2/m$ | – | $2'/m'2/m2'/m'$, $4'/m$ | $\left(\frac{6^{(3)}}{m}\right)^{(3)}$ | $\left(\bar{3}^{(3)}\frac{2^{(2,1)}}{m^{(2,1)}}\right)^{(3)}$ |
| $222$ | $2/m'2/m'2/m'$ | $4'22'$, $\bar{4}'2m'$, | $(23^{(3)})^{(3)}$ | $(6^{(3)}2^{(2,1)}2^{(2,1)})^{(3)}$ |
| $mm2$ | $2'/m2'/m2/m'$ | $4'mm'$, $\bar{4}'m2'$, $\bar{6}'m2'$, $6'mm'$ | – | $(6^{(3)}m^{(2,1)}m^{(2,1)})^{(3)}$, $(\bar{6}^{(3)}m^{(2,1)}2^{(2,1)})^{(3)}$ |
| $2/m2/m2/m$ | – | $4'/m2/m2'/m'$ | $\left(\frac{2}{m}3^{(3)}\right)^{(3)}$ | $\left(\frac{6^{(3)}}{m}\frac{2^{(2,1)}}{m^{(2,1)}}\frac{2^{(2,1)}}{m^{(2,1)}}\right)^{(3)}$ |
| $4$ | $4m'm'$, $4/m'$, $42'2'$ | – | – | – |
| $\bar{4}$ | $4/m'$, $\bar{4}2'm'$ | – | – | – |
| $4/m$ | $4/m2'/m'2'/m'$ | – | – | – |
| $4mm$ | $4/m'2'/m2'/m$ | – | – | – |
| $\bar{4}2m$ | $4/m'2/m'2'/m$ | – | – | $(\bar{4}^{(2,1)}3^{(3)}m^{(2,1)})^{(3)}$ |
| $\bar{4}m2$ | $4/m'2'/m2/m'$ | – | – | |
| $422$ | $4/m'2/m'2/m'$ | – | – | $(4^{(2,1)}3^{(3)}2^{(2,1)})^{(3)}$ |
| $4/m2/m2/m$ | – | – | – | $\left(\frac{4^{(2,1)}}{m}\bar{3}^{(3)}\frac{2^{(2,1)}}{m^{(2,1)}}\right)^{(3)}$ |
| $3$ | $\bar{3}'$, $31m'$, $3m'1$, $312'$, $32'1$ $6'$, $\bar{6}'$ ($\mathbf{L}_{\mathrm{I}} = hP$) | $6'$, $\bar{6}'$ ($\mathbf{L}_{\mathrm{I}} = hR$) | – | $(2^{(2)}3^{(3,1)})^{(4)}$ |
| $\bar{3}$ | $\bar{3}2'/m'1$, $\bar{3}12'/m'$, $6'/m'$ ($\mathbf{L}_{\mathrm{I}} = hP$) | $6'/m'$ ($\mathbf{L}_{\mathrm{I}} = hR$) | – | $\left(\frac{2^{(2)}}{m^{(2)}}\bar{3}^{(3,1)}\right)^{(4)}$ |
| $3m1$ | $\bar{3}'12'/m$, $6'mm'$, $\bar{6}'m2'$ | – | – | $(\bar{4}^{(4)}3^{(3,1)}m^{(2,2)})^{(4)}$ |
| $31m$ | $\bar{3}'2'/m1$, $6'm'm$, $\bar{6}'2'm$ | – | – | |
| $3m$ | $\bar{3}'2'/m$ | $6'mm'$, $\bar{6}'m2'$ | – | |
| $321$ | $\bar{3}'2/m'1$, $6'22'$, $\bar{6}'2m'$ | – | – | $(4^{(4)}3^{(3,1)}2^{(2,2)})^{(4)}$ |
| $312$ | $\bar{3}'12/m'$, $6'2'2$, $\bar{6}'m'2$ | – | – | |
| $32$ | $\bar{3}'2/m$ | $6'22'$, $\bar{6}'2m'$ | – | |
| $\bar{3}2/m1$ | $6'/m'2/m2'/m'$ | – | – | $\left(\frac{4^{(4)}}{m^{(2)}}\bar{3}^{(3,1)}\frac{2^{(2,2)}}{m^{(2,2)}}\right)^{(4)}$ |
| $\bar{3}12/m$ | $6'/m'2'/m'2/m$ | – | – | |
| $\bar{3}2/m$ | – | $6'/m'2'/m'2/m$ | – | |
| $6$ | $6/m'$, $6m'm'$, $62'2'$ | – | – | – |
| $\bar{6}$ | $6'/m$, $\bar{6}2'm'$, $\bar{6}m'2'$ | – | – | – |
| $6/m$ | $6/m2'/m'2'/m'$ | – | – | – |
| $6mm$ | $6/m'2'/m2'/m$ | – | – | – |

**Table 1.** (Continued).

| $\mathcal{H}$ | $\mathcal{K}^{(p)}$ | | | |
|---|---|---|---|---|
| | Twinning by syngonic merohedry: Shubnikov groups $\mathcal{K}^{(2)}$ | Twinning by metric merohedry or by reticular merohedry | | |
| | | Shubnikov groups $\mathcal{K}^{(2)}$ | Koptsik groups $\mathcal{K}^{(p>2)}$ | Van der Waerden-Burckhardt groups $\mathcal{K}_{WB}{}^{(p>2)}$ |
| $\bar{6}2m$ | $6'/m2/m'2'/m$ | – | – | – |
| $\bar{6}m2$ | $6'/m2'/m2/m'$ | – | – | – |
| 622 | $6/m'2/m'2/m'$ | – | – | – |
| $6/m2/m2/m$ | – | – | – | – |
| 23 | $2/m'3'$, $\bar{4}'3m'$, $4'32'$ | $31m'$, $312'$, $6'$, $\bar{6}'$ | – | – |
| $2/m\bar{3}$ | $4'/m\bar{3}2'/m'$ | $\bar{3}12'/m'$, $6'/m'$ | – | – |
| $\bar{4}3m$ | $4'/m'\bar{3}'2'/m$ | $6'mm'$, $\bar{6}'m2'$ | – | – |
| 432 | $4/m'\bar{3}'2/m'$ | $6'22'$, $\bar{6}'2m'$ | – | – |
| $4/m\bar{3}2/m$ | – | $6'/m'2/m2'/m'$ | – | – |

2 totally chromatic elements (with one chromatic index $p_i$): twin elements which do not leave fixed any of the individuals, but exchange all the $p$ individuals in groups of $p_i$; the prime in Shubnikov groups is equivalent to $p_i = 2$;

3 partially chromatic elements: twin elements with two chromatic indices, $p_1, p_2$, which exchange a subset of the individuals, leaving unchanged the others. They are subdivided in two types:

3.1 $p_2 \neq 0$, $p_1 + p_2 \leq p$: symmetry elements for the individual, which leave fixed $p_2$ individuals and exchange the other $p - p_2$ individuals in groups of $p_1$;

3.2 $p_2 = 0$, $3 < p_1 < p$: in cubic twin point groups, symmetry elements for the individual parallel to a twin element. $p_1$ coincides with the geometric order of the twin element and is twice the order of the symmetry element ($4^{(4,0)}$ for $4 \,//\, 2$; $\bar{3}^{(6,0)}$ for $\bar{3} \,//\, 3$). Odd powers of the twin operation exchange all the $p$ individuals, leaving fixed $p_2 = 0$ individuals; even powers of the twin operation correspond to a symmetry operations for the individual, and thus do not act on it: they however act on $mp_1$ individuals but leave fixed the other $p - m \cdot p_1$ individuals, where $m = \text{int}\,(p/p_1)$, "int" standing for "integer".

By applying these criteria, the symmetry of the twin and of the individual are easily derived, as shown in the following examples. The complete list is given in Table 3.

### Example 1. $(6^{(6)}m^{(2,2)}m^{(2)})^{(6)}$

The global chromaticity is $p = 6$, thus this group represents a twin of six individuals. To identify the symmetry of the individual we have to look for achromatic or partially chromatic elements. In this case, no achromatic element exists, while there is one partially chromatic element, $m^{(2,2)}$. The monochromatic point group is thus $\mathcal{H} = m$, which is related to $(6^{(6)}m^{(2,2)}m^{(2)})^{(6)}$ by two independent elements, $3 \,//\, m$ and $2 \,//\, 3$ (see Table 3): this is thus a manifold second-degree twin. The first twin element forms an intermediate first-degree three-chromatic group, whose symbol is $(3^{(3)}m^{(2,1)})^{(3)}$ (cfr. Table 1); the second twin element transforms $3^{(3)}$ in $6^{(6)}$ giving the final symbol $(6^{(6)}m^{(2,2)}m^{(2)})^{(6)}$.

The action of the twin elements is shown in Fig. 1, where the $m$ symmetry of the original individual A is indicated by a segment perpendicular to the mirror. The $6^{(6)}$ axis permutes all the six individuals and is thus totally chromatic. The (01.0) plane becomes partially chromatic, and is thus shown dotted: it leaves fixed the $p_2 = 2$ individuals A and D, and exchanges $p - p_2 = 4$ individuals in groups of $p_1 = 2$: B with F, and C with E. The same partial chromatic nature is acquired by the two other planes generated by the action of $6^{(6)}$ axis on (01.0): (10.0) and (11.0). Finally, the three other (non independent) twin planes are totally chromatic: they exchange all the six individuals in groups of 2.

### Example 2. $\left(\dfrac{2^{(2)}}{m^{(2)}}\,\bar{3}^{(6,0)}\right)^{(8)}$

The global chromaticity is $p = 8$, thus this group represents a twin of eight individuals. Here there is only one partially chromatic element and no achromatic elements: the symmetry of the individual is thus 3 (the ratio of the orders of the groups $2/m\bar{3}$ and 3 is 8, which corresponds to the chromaticity of the group). The first stage of twinning corresponds to the action of the twofold axes diagonal to 3 (parallel to $\langle 001 \rangle$ in the cubic setting of the final group) which equivalent under the action of $3_{[111]}$ and produce the intermediate twin point group $(23^{(3)})^{(3)}$. The second stage of twinning adds the inversion centre. Odd powers of the 3 operation exchange all the eight crystals; even powers correspond to the three-fold rotation, which

**Table 2.** Polychromatic point groups for higher-degree twins. I. $\mathcal{K}^{(p)}$ groups. The sequence of twin elements follows – whenever possible – the sequence of symmorphic space-group type generators, as given in the *International Tables for Crystallography*, vol. A, 5th Edition (cfr. also Fig. 10.1.3.2 in Hahn and Klapper, 2002). For non-cubic groups, the relative disposition of symmetry and twin elements are given; for cubic groups, the absolute directions are instead indicated.

| $\mathcal{K}^{(p)}$ | degree | $\mathcal{H}$ | 1st twin element | 2nd twin element | 3rd twin element | 4th twin element | 5th twin element |
|---|---|---|---|---|---|---|---|
| $\left(\frac{2^{(2)}}{m^{(2)}}\right)^{(4)}$ | 2 | 1 | 2 | $\bar{1}$ | – | – | – |
| $(2^{(2)}2^{(2)}2^{(2)})^{(4)}$ | 2 | 1 | 2 | $2 \perp 2$ | – | – | – |
| $(m^{(2)}m^{(2)}2^{(2)})^{(4)}$ | 2 | 1 | 2 | $m$ // 2 | – | – | – |
| $\left(\frac{2^{(2)}}{m^{(2)}}\frac{2^{(2)}}{m^{(2)}}\frac{2^{(2)}}{m^{(2)}}\right)^{(4)}$ | 2 | $\bar{1}$ | 2 | $2 \perp 2$ | – | – | – |
| $\left(\frac{2^{(2)}}{m^{(2)}}\frac{2}{m^{(2)}}\frac{2^{(2)}}{m^{(2)}}\right)^{(4)}$ | 2 | 2 | $2 \perp 2$ | $\bar{1}$ | – | – | – |
| $\left(\frac{2^{(2)}}{m^{(2)}}\frac{2^{(2)}}{m}\frac{2^{(2)}}{m^{(2)}}\right)^{(4)}$ | 2 | $m$ | 2 // $m$ | $\bar{1}$ | – | – | – |
| $\left(\frac{2^{(2)}}{m^{(2)}}\frac{2^{(2)}}{m^{(2)}}\frac{2^{(2)}}{m^{(2)}}\right)^{(8)}$ | 3 | 1 | 2 | $2 \perp 2$ | $\bar{1}$ | – | – |
| $\left(\frac{4^{(4)}}{m^{(2)}}\right)^{(4)}$ | 2 | $\bar{1}$ | 2 | 4 // 2 | – | – | – |
| $\left(\frac{4^{(4)}}{m}\right)^{(4)}$ | 2 | $m$ | $2 \perp m$ | 4 // 2 | – | – | – |
| $\left(\frac{4^{(2)}}{m^{(2)}}\right)^{(4)}$ | 2 | 2 | 4 // 2 | $\bar{1}$ | – | – | – |
| $\left(\frac{4^{(4)}}{m^{(2)}}\right)^{(8)}$ | 3 | 1 | 2 | 4 // 2 | $\bar{1}$ | – | – |
| $(4^{(2)}2^{(2)}2^{(2)})^{(4)}$ | 2 | 2 (2 // 4) | $2 \perp 2$ | 4 // 2 | – | – | – |
| $(4^{(4)}2^{(2)}2^{(2)})^{(8)}$ | 3 | 1 | 2 | 4 // 2 | $2 \perp 4$ | – | – |
| $(4^{(2)}m^{(2)}m^{(2)})^{(4)}$ | 2 | 2 (2 // 4) | 4 // 2 | $m \perp 2$ | – | – | – |
| $(4^{(4)}m^{(2)}m^{(2)})^{(8)}$ | 3 | 1 | 2 | 4 // 2 | $m$ | – | – |
| $(\bar{4}^{(2)}2^{(2)}m^{(2)})^{(4)}$ | 2 | 2 (2 // 4) | $\bar{4}$ // 2 | $2 \perp 4$ | – | – | – |
| $(\bar{4}^{(4)}2^{(2)}m^{(2)})^{(8)}$ | 3 | 1 | 2 | $\bar{4}$ // 2 | $2 \perp 4$ | – | – |
| $\left(\frac{4}{m^{(2)}}\frac{2^{(2)}}{m^{(2)}}\frac{2^{(2)}}{m^{(2)}}\right)^{(4)}$ | 2 | 4 | $2 \perp 4$ | $\bar{1}$ | – | – | – |
| $\left(\frac{4^{(2)}}{m^{(2)}}\frac{2^{(2)}}{m^{(2)}}\frac{2^{(2)}}{m^{(2)}}\right)^{(4)}$ | 2 | $\bar{4}$ | $2 \perp 4$ | $\bar{1}$ | – | – | – |
| $\left(\frac{4^{(2)}}{m^{(2)}}\frac{2}{m^{(2)}}\frac{2^{(2)}}{m^{(2)}}\right)^{(4)}$ | 2 | 222 | 4 | $\bar{1}$ | – | – | – |
| $\left(\frac{4^{(2)}}{m^{(2)}}\frac{2^{(2)}}{m}\frac{2^{(2)}}{m^{(2)}}\right)^{(4)}$ | 2 | $mm2$ | 4 // 2 | $\bar{1}$ | – | – | – |
| $\left(\frac{4^{(2)}}{m}\frac{2^{(2)}}{m^{(2)}}\frac{2^{(2)}}{m^{(2)}}\right)^{(4)}$ | 2 | $2/m$ | 2 // $m$ | 4 // 2 | – | – | – |
| $\left(\frac{4^{(4)}}{m^{(2)}}\frac{2^{(2)}}{m^{(2)}}\frac{2^{(2)}}{m^{(2)}}\right)^{(8)}$ | 3 | $\bar{1}$ | 2 | 4 // 2 | $2 \perp 4$ | – | – |
| $\left(\frac{4^{(2)}}{m^{(2)}}\frac{2^{(2)}}{m^{(2)}}\frac{2^{(2)}}{m^{(2)}}\right)^{(8)}$ | 3 | 2 | 4 // 2 | $2 \perp 4$ | $\bar{1}$ | – | – |
| $\left(\frac{4^{(4)}}{m}\frac{2^{(2)}}{m^{(2)}}\frac{2^{(2)}}{m^{(2)}}\right)^{(8)}$ | 3 | $m$ | $2 \perp m$ | 2 // $m$ | 4 // 2 | – | – |
| $\left(\frac{4^{(4)}}{m^{(2)}}\frac{2^{(2)}}{m^{(2)}}\frac{2^{(2)}}{m^{(2)}}\right)^{(16)}$ | 4 | 1 | 2 | 4 // 2 | $2 \perp 4$ | $\bar{1}$ | – |
| $\bar{3}^{(6)}$ | 2 | 1 | 3 | $\bar{1}$ | – | – | – |

**Table 2.** (Continued)

| $\mathcal{K}^{(p)}$ | degree | $\mathcal{H}$ | 1st twin element | 2nd twin element | 3rd twin element | 4th twin element | 5th twin element |
|---|---|---|---|---|---|---|---|
| $(3^{(3)}2^{(2)})^{(6)}$ | 2 | 1 | 3 | $2 \perp 3$ | – | – | – |
| $(\bar{3}^{(3)}m^{(2)})^{(6)}$ | 2 | 1 | 3 | $m \,//\, 3$ | – | – | – |
| $(\bar{3}^{(2)}m^{(2)})^{(4)}$ | 2 | 3 | $2 \perp 3$ | $\bar{1}$ | – | – | – |
| $(\bar{3}^{(3)}m^{(2)})^{(6)}$ | 2 | $\bar{1}$ | 3 | $2 \perp 3$ | – | – | – |
| $(\bar{3}^{(6)}m^{(2)})^{(12)}$ | 3 | 1 | 3 | $2 \perp 3$ | $\bar{1}$ | – | – |
| $6^{(6)}$ | 2 | 1 | 3 | $2 \perp 3$ | – | – | – |
| $\bar{6}^{(6)}$ | 2 | 1 | 3 | $m \perp 3$ | – | – | – |
| $\left(\frac{6^{(2)}}{m^{(2)}}\right)^{(4)}$ | 2 | 3 | $2 \,//\, 3$ | $\bar{1}$ | – | – | – |
| $\left(\frac{6^{(3)}}{m^{(2)}}\right)^{(6)}$ | 2 | 2 | $3 \,//\, 2$ | $\bar{1}$ | – | – | – |
| $\left(\frac{6^{(6)}}{m^{(2)}}\right)^{(6)}$ | 2 | $\bar{1}$ | 3 | $2 \,//\, 3$ | – | – | – |
| $\left(\frac{6^{(6)}}{m}\right)^{(6)}$ | 2 | $m$ | $3 \perp m$ | $2 \,//\, 3$ | – | – | – |
| $\left(\frac{6^{(6)}}{m^{(2)}}\right)^{(12)}$ | 3 | 1 | 3 | $2 \,//\, 3$ | $\bar{1}$ | – | – |
| $(6^{(2)}2^{(2)}2^{(2)})^{(4)}$ | 2 | 3 | $2 \,//\, 3$ | $2 \perp 3$ | – | – | – |
| $(6^{(3)}2^{(2)}2^{(2)})^{(6)}$ | 2 | 2 | $3 \,//\, 2$ | $2 \perp 3$ | – | – | – |
| $(6^{(6)}2^{(2)}2^{(2)})^{(12)}$ | 3 | 1 | 3 | $2 \,//\, 3$ | $2 \perp 6$ | – | – |
| $(6^{(2)}m^{(2)}m^{(2)})^{(4)}$ | 2 | 3 | $2 \,//\, 3$ | $m \,//\, 3$ | – | – | – |
| $(6^{(3)}m^{(2)}m^{(2)})^{(6)}$ | 2 | 2 | $3 \,//\, 2$ | $m \,//\, 3$ | – | – | – |
| $(6^{(6)}m^{(2)}m^{(2)})^{(12)}$ | 3 | 1 | 3 | $2 \,//\, 3$ | $m \,//\, 3$ | – | – |
| $(\bar{6}^{(2)}m^{(2)}2^{(2)})^{(4)}$ | 2 | 3 | $m \,//\, 3$ | $2 \perp 3$ | – | – | – |
| $(\bar{6}^{(3)}m2^{(2)})^{(6)}$ | 2 | $m_1$ | 3 | $m_2$ | – | – | – |
| $(\bar{6}^{(6)}m^{(2)}2^{(2)})^{(12)}$ | 3 | 1 | 3 | $m_1$ | $m_2$ | – | – |
| $\left(\frac{6^{(2)}}{m^{(2)}}\frac{2^{(2)}}{m^{(2)}}\frac{2^{(2)}}{m^{(2)}}\right)^{(4)}$ | 2 | $\bar{3}$ | $2 \,//\, 3$ | $2 \perp 3$ | – | – | – |
| $\left(\frac{6^{(2)}}{m^{(2)}}\frac{2}{m^{(2)}}\frac{2^{(2)}}{m^{(2)}}\right)^{(4)}$ | 2 | 32 | $2 \,//\, 3$ | $\bar{1}$ | – | – | – |
| $\left(\frac{6^{(2)}}{m^{(2)}}\frac{2^{(2)}}{m}\frac{2^{(2)}}{m^{(2)}}\right)^{(4)}$ | 2 | $3m$ | $2 \,//\, 3$ | $\bar{1}$ | – | – | – |
| $\left(\frac{6}{m^{(2)}}\frac{2^{(2)}}{m^{(2)}}\frac{2^{(2)}}{m^{(2)}}\right)^{(4)}$ | 2 | 6 | $2 \perp 6$ | $\bar{1}$ | – | – | – |
| $\left(\frac{6^{(2)}}{m}\frac{2^{(2)}}{m^{(2)}}\frac{2^{(2)}}{m^{(2)}}\right)^{(4)}$ | 2 | $\bar{6}$ | $2 \,//\, 3$ | $2 \perp 6$ | – | – | – |
| $\left(\frac{6^{(3)}}{m}\frac{2^{(2)}}{m^{(2)}}\frac{2^{(2)}}{m^{(2)}}\right)^{(6)}$ | 2 | $2/m$ | $3 \,//\, 2$ | $2 \perp 6$ | – | – | – |
| $\left(\frac{6^{(2)}}{m^{(2)}}\frac{2^{(2)}}{m^{(2)}}\frac{2^{(2)}}{m^{(2)}}\right)^{(8)}$ | 3 | 3 | $2 \,//\, 3$ | $2 \perp 3$ | $\bar{1}$ | – | – |
| $\left(\frac{6^{(6)}}{m^{(2)}}\frac{2^{(2)}}{m^{(2)}}\frac{2^{(2)}}{m^{(2)}}\right)^{(12)}$ | 3 | $\bar{1}$ | 3 | $2 \,//\, 3$ | $2 \perp 3$ | – | – |
| $\left(\frac{6^{(3)}}{m^{(2)}}\frac{2^{(2)}}{m^{(2)}}\frac{2^{(2)}}{m^{(2)}}\right)^{(12)}$ | 3 | 2 | $3 \,//\, 2$ | $2 \perp 3$ | $\bar{1}$ | – | – |
| $\left(\frac{6^{(6)}}{m}\frac{2^{(2)}}{m^{(2)}}\frac{2^{(2)}}{m^{(2)}}\right)^{(12)}$ | 3 | $m$ | $3 \perp m$ | $2 \,//\, 3$ | $2 \perp 3$ | – | – |

**Table 2.** (Continued)

| $\mathcal{K}^{(p)}$ | degree | $\mathcal{H}$ | 1st twin element | 2nd twin element | 3rd twin element | 4th twin element | 5th twin element |
|---|---|---|---|---|---|---|---|
| $\left(\frac{6^{(6)}}{m^{(2)}}\frac{2^{(2)}}{m^{(2)}}\frac{2^{(2)}}{m^{(2)}}\right)^{(24)}$ | 4 | 1 | 3 | 2 // 3 | $2 \perp 3$ | $\bar{1}$ | – |
| $(2^{(2)}3^{(3)})^{(12)}$ | 3 | 1 | $2_{[001]}$ | $2_{[010]}$ | $3_{[111]}$ | – | – |
| $\left(\frac{2}{m^{(2)}}\bar{3}^{(6)}\right)^{(6)}$ | 2 | 222 | $3_{[111]}$ | $\bar{1}$ | – | – | – |
| $\left(\frac{2^{(2)}}{m^{(2)}}\bar{3}^{(3)}\right)^{(12)}$ | 3 | $\bar{1}$ | $2_{[001]}$ | $2_{[010]}$ | $3_{[111]}$ | – | – |
| $\left(\frac{2^{(2)}}{m^{(2)}}\bar{3}^{(6)}\right)^{(24)}$ | 4 | 1 | $2_{[001]}$ | $2_{[010]}$ | $3_{[111]}$ | $\bar{1}$ | – |
| $(4^{(4)}3^{(3)}2^{(2)})^{(6)}$ | 2 | 222 | $3_{[111]}$ | $2_{[110]}$ | – | – | – |
| $(4^{(4)}3^{(3)}2^{(2)})^{(24)}$ | 4 | 1 | $2_{[001]}$ | $2_{[010]}$ | $3_{[111]}$ | $2_{[110]}$ | – |
| $(4^{(2)}3^{(3)}m^{(2)})^{(6)}$ | 2 | 222 | $3_{[111]}$ | $m_{xxz}$ | – | – | – |
| $(\bar{4}^{(4)}3^{(3)}m^{(2)})^{(24)}$ | 4 | 1 | $2_{[001]}$ | $2_{[010]}$ | $3_{[111]}$ | $m_{xxz}$ | – |
| $\left(\frac{4^{(2)}}{m^{(2)}}\bar{3}^{(2)}\frac{2^{(2)}}{m^{(2)}}\right)^{(4)}$ | 2 | 23 | $2_{[110]}$ | $\bar{1}$ | – | – | – |
| $\left(\frac{4^{(2)}}{m}\bar{3}^{(3)}\frac{2^{(2)}}{m^{(2)}}\right)^{(6)}$ | 2 | *mmm* | $3_{[111]}$ | $\bar{1}$ | – | – | – |
| $\left(\frac{4^{(2)}}{m^{(2)}}\bar{3}^{(6)}\frac{2^{(2)}}{m^{(2)}}\right)^{(12)}$ | 3 | 222 | $3_{[111]}$ | $2_{[110]}$ | $\bar{1}$ | – | – |
| $\left(\frac{4^{(4)}}{m^{(2)}}\bar{3}^{(3)}\frac{2^{(2)}}{m^{(2)}}\right)^{(24)}$ | 4 | $\bar{1}$ | $2_{[001]}$ | $2_{[010]}$ | $3_{[111]}$ | $2_{[110]}$ | – |
| $\left(\frac{4^{(4)}}{m^{(2)}}\bar{3}^{(6)}\frac{2^{(2)}}{m^{(2)}}\right)^{(48)}$ | 5 | 1 | $2_{[001]}$ | $2_{[010]}$ | $3_{[111]}$ | $2_{[110]}$ | $\bar{1}$ |

are symmetry operations for the individual: they keep fixed $8 - 6 = 2$ individuals, and exchange the other 6 individuals. The twofold axes and the mirror are totally chromatic.

## TLQS twinning

For these twins, the polychromatic point group represents the *approximate* symmetry of the twin, the degree of approximation being measured by the obliquity. However, the twin *elements* may need a slightly modified notation. Donnay and Donnay (1974) have proposed to use a dashed fraction bar to indicate nearly perpendicularity between twin axis and twin plane (*n*/*m*) instead of the solid fraction bar expressing perpendicularity (*n*/*m*). The same notation can be extended to polychromatic groups. The twin centre is no longer implied, even for axes of even order; if present, it has to be explicitly given in the symbol.

## The symmetry of the incomplete twin: manifold twin operation as *partial* operation

Sadanaga et al. (1980) have defined a superstructure as a structure consisting of substructures (nearly) equal to each other in configuration, each substructure being related to another substructure by an operation (a motion) which can be of three types: 1) a *global symmetry operation*, effective everywhere in the crystal space (an ordinary space-group operation); 2) a *local symmetry operation*, effective only within a certain subspace of the crystal space and bringing the subspace to superpose upon itself (a space-groupoid operation); 3) a *partial operation*, effective only within a subspace of the crystal space and bringing the subspace to superpose upon another subspace. A partial operation $\varphi$ is a non-symmetry operation inasmuch that $\varphi(\mathrm{A}) = \mathrm{B}$ while $\varphi(\mathrm{B})$ is undefined ("supersymmetry" according to Zorkii, 1978).

There is clearly a parallel between superstructure vs. its substructures on one side, and twin vs. its individuals on the other side. The totally chromatic operations are effective on all the individuals of the twin and in this respect they play the same role of global symmetry operations in superstructures. The partially chromatic operations are symmetry operations for one individual, but exchange the other individuals: in this respect they play the same role of local symmetry operations in superstructures.

In case of manifold twins, Eq. (1), which gives the twin multiplicity, may be satisfied for $m < m'$. The number of individuals related by at least one manifold twin element is lower than the chromaticity of that element. There can be several reasons for one or more individuals miss-

**Table 3.** Polychromatic point groups for higher-degree twins. II. $\mathcal{K}_{WB}^{(p)}$ groups. $2_d$ indicates two-fold axis diagonal with respect to the 3 fold axis of the individual (parallel to $\langle 100\rangle$ in the cubic setting of the polychromatic group). The orientation of the symmetry elements of $\mathcal{H}$, when not explicitly given, can be derived from the orientation of partially chromatic elements in $\mathcal{K}_{WB}^{(p)}$. Other conventions as in Table 2.

| $\mathcal{K}_{WB}^{(p)}$ | degree | $\mathcal{H}$ | 1st twin element | 2nd twin element | 3rd twin element | 4th twin element |
|---|---|---|---|---|---|---|
| $(4^{(4)}2^{(2,2)}2^{(2)})^{(4)}$ | 2 | $2\ (2 \perp 4)$ | $2 \perp 2$ | 4 | – | – |
| $(4^{(4)}m^{(2,2)}m^{(2)})^{(4)}$ | 2 | $m$ | $2\ //\ m$ | $4\ //\ 2$ | – | – |
| $(\bar{4}^{(4)}2^{(2,2)}m^{(2)})^{(4)}$ | 2 | 2 | $\bar{4}\ //\ 2$ | $2 \perp 4$ | – | – |
| $(\bar{4}^{(4)}2^{(2)}m^{(2,2)})^{(4)}$ | 2 | $m$ | 2 | $\bar{4}\ //\ 2$ | – | – |
| $\left(\frac{4^{(4)}}{m}\frac{2^{(2.2)}}{m^{(2.2)}}\frac{2^{(2)}}{m^{(2)}}\right)^{(4)}$ | 2 | $mm2\ (2 \perp 4)$ | $4\ //\ 2$ | $\bar{1}$ | – | – |
| $\left(\frac{4^{(4)}}{m^{(2)}}\frac{2^{(2.2)}}{m^{(2.2)}}\frac{2^{(2)}}{m^{(2)}}\right)^{(4)}$ | 2 | $2/m$ | $2\ //\ m$ | $4\ //\ 2$ | – | – |
| $\left(\frac{4^{(4)}}{m^{(2)}}\frac{2^{(2,4)}}{m^{(2)}}\frac{2^{(2)}}{m^{(2)}}\right)^{(8)}$ | 3 | 2 | $4\ //\ 2$ | $2 \perp 4$ | $\bar{1}$ | – |
| $\left(\frac{4^{(4)}}{m^{(2)}}\frac{2^{(2)}}{m^{(2,4)}}\frac{2^{(2)}}{m^{(2)}}\right)^{(8)}$ | 3 | $m$ | $4\ //\ m$ | $2 \perp 4$ | $\bar{1}$ | – |
| $\left(\bar{3}^{(6)}\frac{2^{(2,2)}}{m^{(2)}}\right)^{(6)}$ | 2 | 2 | $3\ //\ 2$ | $\bar{1}$ | – | – |
| $\left(\bar{3}^{(6)}\frac{2^{(2)}}{m^{(2,2)}}\right)^{(6)}$ | 2 | $m$ | $3 \perp m$ | $\bar{1}$ | – | – |
| $(6^{(6)}2^{(2,2)}2^{(2)})^{(6)}$ | 2 | 2 | $3\ //\ 2$ | $2 \perp 6$ | – | – |
| $(6^{(6)}m^{(2,2)}m^{(2)})^{(6)}$ | 2 | $m$ | 3 | $2\ //\ 3$ | – | – |
| $(\bar{6}^{(6)}m^{(2)}2^{(2,2)})^{(6)}$ | 2 | 2 | 3 | $m\ //\ 2$ | – | – |
| $(\bar{6}^{(6)}m^{(2,2)}2^{(2)})^{(6)}$ | 2 | $m_1$ | 3 | $m_2$ | – | – |
| $\left(\frac{6^{(3)}}{m^{(2)}}\frac{2^{(2,2)}}{m^{(2)}}\frac{2^{(2,2)}}{m^{(2)}}\right)^{(6)}$ | 2 | 222 | 3 | $\bar{1}$ | – | – |
| $\left(\frac{6^{(3)}}{m^{(2)}}\frac{2^{(2)}}{m^{(2,2)}}\frac{2^{(2)}}{m^{(2,2)}}\right)^{(6)}$ | 2 | $mm2\ (2\ //\ 6)$ | 3 | $\bar{1}$ | – | – |
| $\left(\frac{6^{(6)}}{m}\frac{2^{(2)}}{m^{(2,2)}}\frac{2^{(2)}}{m^{(2)}}\right)^{(6)}$ | 2 | $mm2\ (2 \perp 6)$ | 3 | $\bar{1}$ | – | – |
| $\left(\frac{6^{(6)}}{m^{(2)}}\frac{2^{(2,2)}}{m^{(2,2)}}\frac{2^{(2)}}{m^{(2)}}\right)^{(6)}$ | 2 | $2/m$ | $3 \perp 2$ | $2\ //\ 3$ | – | – |
| $\left(\frac{6^{(6)}}{m^{(2)}}\frac{2^{(2,4)}}{m^{(2)}}\frac{2^{(2)}}{m^{(2)}}\right)^{(12)}$ | 3 | 2 | $2 \perp 2$ | 3 | $\bar{1}$ | – |
| $\left(\frac{6^{(6)}}{m^{(2)}}\frac{2^{(2)}}{m^{(2,4)}}\frac{2^{(2)}}{m^{(2)}}\right)^{(12)}$ | 3 | $m$ | $2\ //\ m$ | $3\ //\ 2$ | $\bar{1}$ | – |
| $(2^{(2,2)}3^{(3)})^{(6)}$ | 2 | 2 | $2_{[001]}$ | $3_{[111]}$ | – | – |
| $\left(\frac{2^{(2,2)}}{m^{(2,2)}}\bar{3}^{(3)}\right)^{(6)}$ | 2 | $2/m$ | $2_{[001]}$ | $3_{[111]}$ | – | – |
| $\left(\frac{2^{(2,2)}}{m^{(2,4)}}\bar{3}^{(6)}\right)^{(6)}$ | 2 | $mm2$ | $3_{[111]}$ | $\bar{1}$ | – | – |
| $\left(\frac{2^{(2)}}{m^{(2)}}\bar{3}^{(6,0)}\right)^{(8)}$ | 2 | 3 | $2_d$ | $\bar{1}$ | – | – |
| $\left(\frac{2^{(2,4)}}{m^{(2)}}\bar{3}^{(6)}\right)^{(12)}$ | 3 | 2 | $2_{[001]}$ | $3_{[111]}$ | $\bar{1}$ | – |
| $\left(\frac{2^{(2)}}{m^{(2,4)}}\bar{3}^{(6)}\right)^{(12)}$ | 3 | $m$ | $2_{[001]}$ | $3_{[111]}$ | $\bar{1}$ | – |
| $(4^{(4,2)}3^{(3)}2^{(2)})^{(6)}$ | 2 | 4 | $3_{[111]}$ | $2_{[110]}$ | – | – |
| $(4^{(4,0)}3^{(3)}2^{(2,2)})^{(6)}$ | 2 | 222 | $3_{[111]}$ | $2_{[110]}$ | – | – |
| $(4^{(4)}3^{(3,2)}2^{(2)})^{(8)}$ | 2 | 3 | $2_{[010]}$ | $2_{[110]}$ | – | – |
| $(4^{(4,0)}3^{(3)}2^{(2)})^{(12)}$ | 3 | $2\ (2\ //\ 4)$ | $2_{[010]}$ | $3_{[111]}$ | $2_{[110]}$ | – |
| $(4^{(4)}3^{(3)}2^{(2,2)})^{(12)}$ | 3 | $2\ (2 \perp 4)$ | $2_{[001]}$ | $3_{[111]}$ | $2_{[110]}$ | – |

**Table 3.** (Continued)

| $\mathcal{K}_{\mathrm{WB}}{}^{(p)}$ | degree | $\mathcal{H}$ | 1st twin element | 2nd twin element | 3rd twin element | 4th twin element |
|---|---|---|---|---|---|---|
| $(4^{(4,2)}3^{(3)}m^{(2)})^{(6)}$ | 2 | $\bar{4}$ | $2_{[010]}$ | $3_{[111]}$ | – | – |
| $(4^{(4,0)}3^{(3)}m^{(2,2)})^{(6)}$ | 2 | $mm2$ | $3_{[111]}$ | $2_{[110]}$ | – | – |
| $(4^{(4)}3^{(3,2)}m^{(2)})^{(8)}$ | 2 | 3 | 4 | $m_{xxz}$ | – | – |
| $(4^{(4,0)}3^{(3)}m^{(2)})^{(12)}$ | 3 | 2 (2 // 4) | $2_{[001]}$ | $3_{[111]}$ | $m_{xxz}$ | – |
| $(4^{(4)}3^{(3)}m^{(2,2)})^{(12)}$ | 3 | $m$ | $2_{[001]}$ | $2_{[010]}$ | $3_{[111]}$ | – |
| $\left(\frac{4^{(4,2)}}{m^{(2,2)}}\bar{3}^{(3)}\frac{2^{(2)}}{m^{(2)}}\right)^{(6)}$ | 2 | $4/m$ | $2_{[010]}$ | $3_{[111]}$ | – | – |
| $\left(\frac{4^{(4,2)}}{m^{(2,4)}}\bar{3}^{(6)}\frac{2^{(2)}}{m^{(2,2)}}\right)^{(6)}$ | 2 | $4mm$ | $2_{[010]}$ | $3_{[111]}$ | – | – |
| $\left(\frac{4^{(2,2)}}{m^{(2)}}\bar{3}^{(6)}\frac{2^{(2,2)}}{m^{(2)}}\right)^{(6)}$ | 2 | 422 | $3_{[111]}$ | $\bar{1}$ | – | – |
| $\left(\frac{4^{(2,2)}}{m^{(2)}}\bar{3}^{(6)}\frac{2^{(2)}}{m^{(2,2)}}\right)^{(6)}$ | 2 | $\bar{4}2m$ | $3_{[111]}$ | $\bar{1}$ | – | – |
| $\left(\frac{4^{(4,0)}}{m^{(2,2)}}\bar{3}^{(3)}\frac{2^{(2,2)}}{m^{(2,2)}}\right)^{(6)}$ | 2 | $mmm$ | $3_{[111]}$ | $2_{[110]}$ | – | – |
| $\left(\frac{4^{(4,0)}}{m^{(2,4)}}\bar{3}^{(6)}\frac{2^{(2,2)}}{m^{(2)}}\right)^{(6)}$ | 2 | $\bar{4}2m$ | $3_{[111]}$ | $\bar{1}$ | – | – |
| $\left(\frac{4^{(4)}}{m^{(2)}}\bar{3}^{(3,2)}\frac{2^{(2)}}{m^{(2)}}\right)^{(8)}$ | 2 | $\bar{3}$ | $2_d$ | $2_{[001]}$ | – | – |
| $\left(\frac{4^{(4)}}{m^{(2)}}\bar{3}^{(6,0)}\frac{2^{(2,4)}}{m^{(2)}}\right)^{(8)}$ | 2 | 32 | $2_{[001]}$ | $\bar{1}$ | – | – |
| $\left(\frac{4^{(4)}}{m^{(2)}}\bar{3}^{(6,0)}\frac{2^{(2)}}{m^{(2,4)}}\right)^{(8)}$ | 2 | $3m$ | $2_{[001]}$ | $\bar{1}$ | – | – |
| $\left(\frac{4^{(4,4)}}{m^{(2)}}\bar{3}^{(6)}\frac{2^{(2)}}{m^{(2)}}\right)^{(12)}$ | 3 | 4 | $2_{[010]}$ | $3_{[111]}$ | $\bar{1}$ | – |
| $\left(\frac{4^{(4,0)}}{m^{(2)}}\bar{3}^{(6)}\frac{2^{(2)}}{m^{(2)}}\right)^{(12)}$ | 3 | $\bar{4}$ | $2_{[100]}$ | $3_{[111]}$ | $\bar{1}$ | – |
| $\left(\frac{4^{(4,0)}}{m^{(2)}}\bar{3}^{(6)}\frac{2^{(2,4)}}{m^{(2)}}\right)^{(12)}$ | 3 | 222 | $3_{[111]}$ | $2_{[110]}$ | $\bar{1}$ | – |
| $\left(\frac{4^{(4,0)}}{m^{(2,8)}}\bar{3}^{(6)}\frac{2^{(2)}}{m^{(2)}}\right)^{(12)}$ | 3 | $mm2$, (2 // 4, $m_{\perp[100]}$) | $3_{[111]}$ | $2_{[110]}$ | $\bar{1}$ | – |
| $\left(\frac{4^{(4,0)}}{m^{(2)}}\bar{3}^{(6)}\frac{2^{(2)}}{m^{(2,4)}}\right)^{(12)}$ | 3 | $mm2$ (2 // 4, $m_{\perp[110]}$) | $3_{[111]}$ | $2_{[110]}$ | $\bar{1}$ | – |
| $\left(\frac{4^{(4)}}{m^{(2,4)}}\bar{3}^{(6)}\frac{2^{(2)}}{m^{(2,2)}}\right)^{(12)}$ | 3 | $mm2$ ($2_{//[1\bar{1}0]}$) | $3_{[111]}$ | $2_{[110]}$ | $\bar{1}$ | – |
| $\left(\frac{4^{(4,0)}}{m^{(2,4)}}\bar{3}^{(3)}\frac{2^{(2)}}{m^{(2,2)}}\right)^{(12)}$ | 3 | $2/m$ (2 // 4) | $2_{[010]}$ | $3_{[111]}$ | $2_{[110]}$ | – |
| $\left(\frac{4^{(4)}}{m^{(2)}}\bar{3}^{(3)}\frac{2^{(2)}}{m^{(2)}}\right)^{(12)}$ | 3 | $2/m$ (2 ⊥ 4) | $2_{[010]}$ | $3_{[111]}$ | $2_{[110]}$ | – |
| $\left(\frac{4^{(4)}}{m^{(2)}}\bar{3}^{(6,0)}\frac{2^{(2)}}{m^{(2)}}\right)^{(16)}$ | 3 | 3 | $2_{[001]}$ | $2_{[010]}$ | $2_{[100]}$ | $\bar{1}$ |
| $\left(\frac{4^{(4,0)}}{m^{(2)}}\bar{3}^{(6)}\frac{2^{(2)}}{m^{(2)}}\right)^{(24)}$ | 4 | 2 (2 // 4) | $2_{[010]}$ | $3_{[111]}$ | $2_{[110]}$ | $\bar{1}$ |
| $\left(\frac{4^{(4)}}{m^{(2)}}\bar{3}^{(6)}\frac{2^{(2,4)}}{m^{(2)}}\right)^{(24)}$ | 4 | 2 (2 ⊥ 4) | $2_{[001]}$ | $3_{[111]}$ | $2_{[110]}$ | $\bar{1}$ |
| $\left(\frac{4^{(4)}}{m^{(2,8)}}\bar{3}^{(6)}\frac{2^{(2)}}{m^{(2)}}\right)^{(24)}$ | 4 | $m$ ($m$ ⊥ 4) | $2_{[001]}$ | $3_{[111]}$ | $2_{[110]}$ | $\bar{1}$ |
| $\left(\frac{4^{(4)}}{m^{(2)}}\bar{3}^{(6)}\frac{2^{(2)}}{m^{(2,4)}}\right)^{(24)}$ | 4 | $m$ ($m$ // 4) | $2_{[001]}$ | $3_{[111]}$ | $2_{[110]}$ | $\bar{1}$ |

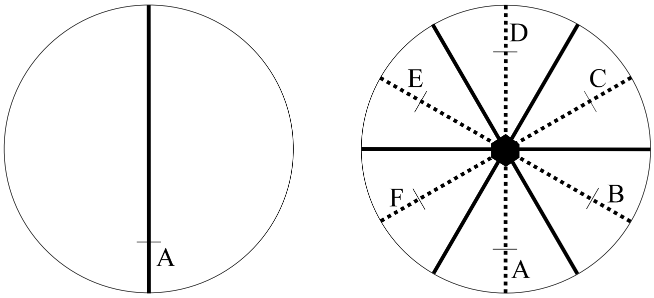


**Fig. 1.** Comparison of $\mathcal{H} = m$ and $\mathcal{K}_{WB}^{(6)} = (6^{(6)}m^{(2,2)}m^{(2)})^{(6)}$ groups. A segment perpendicular to the mirror is used to indicate the *m* eigensymmetry of the individual. In $\mathcal{K}_{WB}^{(6)}$ the original mirror plane, as well as the two others equivalent to it, is dashed to indicate its partial chromaticity. The second set of three mirrors is totally chromatic and drawn thus by solid lines.

ing: mechanical constraints (the twin growing on a surface preventing the development of some individuals), morphological constraints (twin formed by attachment of individuals with relative orientation corresponding to an *n*-fold rotation), accidental events (physical rupture of the twin). For the twin as a whole, the twin operation is no longer a true symmetry operation, but rather a *partial* operation in the meaning explained above. In the case of superstructures, the partial operation does not appear in the symmetry as expressed by the space-group type. For twins, the occasional lack of one or more individuals should not affect the symbol of the twin point group, otherwise the true symmetry of the twin would be hidden. For example, let us compare the $(3^{(3)}2^{(2,1)})^{(3)}$ threefold twin discussed above in the case when one of its individuals is missing, and a twofold twin where the individuals of symmetry 2 are twinned according to a twofold axis bisecting the intercrystal angle (Fig. 2). The symmetry elements of the individuals which are not parallel to each other are either lost in the twin (Buerger, 1954) or become partially chromatic elements if they are related by a totally chromatic twin element of order higher then 2 (see Table 3). The two-individual twin in the central part of Fig. 2 is not a twofold twin, but rather a threefold twin with a missing individual. The thrichromatic axis $3^{(3)}$ still relates the two individuals left: the twin operation about it does not disappear, but is rather transformed into a *partial twin operation*, in the meaning of partial operation discussed above. To indicate this accidental lack of individuals in twins we propose the term *incomplete twinning*. In this respect, the term *complete twin* introduced by Curien and Donnay (1959), which has become practically undefined once the limitation on the crystal family has been removed, is logically redefined to indicate a manifold twin in which none of the twin operations is partial. In higher-degree twins, the complete or incomplete character has to be judged with respect to each intermediate twin point group.

Symbols for incomplete twins are easily obtained from the polychromatic symbols by modifying only the global chromaticity index *p*, which is now split into two parts, a superscript $p_p$ (the lower "*p*" for "present") and a subscript $p_a$ ("*a*" for absent), with the obvious relation between the complete and incomplete twin: $p = p_p + p_a$. In the example above, the symbol of the twin point group becomes simply$(3^{(3)}2^{(2,1)})^{(2)}_{(1)}$.

Fig. 2 shows clearly that this incomplete twin has higher, although partial, symmetry than the $2'$ twin with which it could be easily mistaken.

## Analysis of examples from the literature

$NaBa_2M_2^{2+}M^{3+}O_6$ ($M$ = Ni, Cu) Quarez et al. (2002) is orthorhombic, space-group type *Fmmm* ($\mathcal{H} = mmm$) with a perfectly hexagonal mesh in the (001) plane ($a = 8.296(2)$, $b = 14.369(3)$, $c = 11.225(3)$ Å for $M$ = Ni; $a = 8.416(2)$, $b = 14.577(5)$, $c = 11.418(3)$ Å for $M$ = Cu; $b = a \cdot 3^{1/2}$ in both cases). Based on this hexagonal mesh, a *hP* sublattice exists, which corresponds to the twin lattice. The three-fold axis of this sublattice acts as twin element, producing a threefold first-degree twin. Twinning is by reticular merohedry, twin index 2, described by the $\mathcal{K}_{WB}^{(3)}$ group

$$\left(\frac{6^{(3)}}{m}\ \frac{2^{(2,1)}}{m^{(2,1)}}\ \frac{2^{(2,1)}}{m^{(2,1)}}\right)^{(3)}.$$

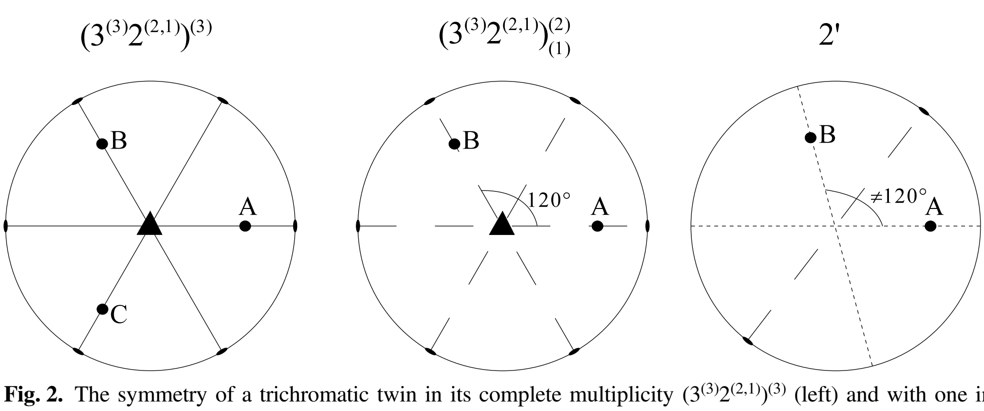


**Fig. 2.** The symmetry of a trichromatic twin in its complete multiplicity $(3^{(3)}2^{(2,1)})^{(3)}$ (left) and with one individual missing $(3^{(3)}2^{(2,1)})^{(2)}_{(1)}$ (centre), and the symmetry of a binary twin $2'$ (right). In all cases, the individuals have symmetry 2. Solid lines are partially chromatic two-fold axes: symmetry elements for one individual, which are also twin elements relating the two other individuals (left). When one individual is missing (centre), their partial chromaticity splits into symmetry component (for the individuals left) and twin component (for the individual missing) (dashed lines). Dotted lines for the $2'$ twin (right) simply indicate the angular separation between the two individuals.

Twinning in $\eta^8$-cyclooctatetraenyl)[hydrotris(pyrazolly) borato]titan(III) was presented by Herbst-Irmer and Sheldrick (1998). The *mC* cell ($a = 10.220$, $b = 11.083$, $c = 7.538$ Å, $\beta = 96.85°$, *Cm*) has a metrically *hR* primitive cell with $a = 7.538$ Å and $\alpha = 94.64°$, and the twin element is $3_{[111]}$ (rhombohedral indexing). Twinning by metric merohedry occurs with respect to $\mathcal{H} = m$ and is described by the trichromatic point group $\mathcal{K}_{WB}{}^{(3)} = (3^{(3)}m^{(2,1)})^{(3)}$. The trichromatic axis $3^{(3)}$ corresponds to symmetry axis for $\mathbf{L}_T$, whereas the *m* plane is partially chromatic: it is a symmetry element for the individual to which it belongs, but at the same time it exchanges the two other individuals.

A similar case of twinning by metric merohedry occurs also in $S_3(Ru_{0.336}Pt_{0.664})\ CuO_6$ (Friese et al., 2003), monoclinic holohedral ($\mathcal{H} = 2/m$) but with a rhombohedral lattice. The trichromatic point group is centrosymmetric, $\mathcal{K}_{WB}{}^{(3)} = \left(\bar{3}^{(3)}\,\frac{2^{(2,1)}}{m^{(2,1)}}\right)^{(3)}$. This compound undergoes further twinning, this time by reticular merohedry with twin index $n_T = 3$. The twin lattice is *hP*, which is a sublattice of *hR*, and twinning by reticular merohedry is described, *with respect to* $\mathbf{L}_I$, by the dichromatic point group $6'/m'2/m2'/m'$. As a whole, with respect to $\mathcal{H} = 2/m$, the second-degree twin symbol is hexachromatic: $\mathcal{K}_{WB}{}^{(6)} = \left(\frac{6^{(6)}}{m}\,\frac{2^{(2,2)}}{m^{(2,2)}}\,\frac{2^{(2)}}{m^{(2)}}\right)^{(6)}$.

The same twinning, described by the same $\mathcal{K}_{WB}{}^{(6)}$ symbol, is shown also by the low temperature (LT) phase of $Cs_3Bi_2I_9$ (Arakcheeva et al., 2001) which is a monoclinic distortion of the hexagonal room temperature (RT) phase (LT: $a = 8.346(6)$, $b = 14.472(9)$, $c = 21.10(1)$ Å, $\beta = 91.00(6)°$, *C2/c*; RT: $a = 8.409(1)$, $c = 21.243(5)$ Å, $P6_3/mmc$). The twin lattice is the hexagonal lattice of the RT phase, and twinning is by pseudo-merohedry. The two lattices have *a* in common, whereas $b_{LT}$ is approximately parallel to $[120]_{RT}$. The unique axis (*c*) of the RT lattice is thus perpendicular to the unique axis (*b*) of the LT lattice. The twin consists of six individuals, which the authors however described as "related by the symmetry operations 3-fold axis and *m*-planes". Actually, the orientation of these twin elements as given by authors [$3 \perp (001)_{LT}$, $m_1 \,//\, (100)_{LT}$, $m_2 \,//\, (001)_{LT}$] shows that the sixfold axis of the RT lattice is totally chromatic, responsible thus for all the six individuals, the other twin elements being not independent.

$Cu_8GeS_6$ (Onoda et al., 1999) is orthorhombic (space-group type $Pmn2_1$) but with a pseudo-tetragonal lattice ($a = 7.0445$, $b = 6.9661$, $c = 9.8699$ Å) and a pseudo-cubic sublattice (*a* close to 9.9 Å and angles close to 90°) that the authors have described as pseudo-rhombohedral.

The first stage of this composite twinning consists in a binary twin by merohedry, the twin element being the inversion centre, for which the authors gave the equivalent $2_{[100]}$ twin axis (domain 4 in table 2 therein). The second stage of twinning consists in a threefold twin by reticular pseudo-merohedry (twin index 2) with respect to the pseudo-cubic sublattice. The number of individuals increases to 6, and the composite twin is described by the hexachromatic point group $\mathcal{K}_{WB}{}^{(6)} = \left(\frac{2^{(2,2)}}{m^{(2,4)}}\,\bar{3}^{(6)}\right)^{(6)}$.

Finally, six other individuals, of smaller size, showed reflections which could not be indexed with integral values, and were refined by using a six-dimensional approach.

## Conclusions

The application of dichromatic point groups to describe the symmetry of twins – approximate in the case of TLQS – has been extended to polychromatic point groups, by means of which multiple and higher-degree twins can be described too by means of a single, compact symbol giving the symmetry of both the twin and the individual. The concepts of *incomplete twin* and of *partial twin operation* have been introduced, to differentiate twins in which one or more individuals are accidentally missing from twins with the same number of individuals but lower symmetry.

The examples discussed, all taken from the recent literature, have shown the need to improve the geminographical knowledge and awareness of the daily crystallographer, who is confronted with twinned crystals and sometimes ends with imprecise descriptions of his samples, even when he succeeds in solving and refining the structure.

*Acknowledgments.* I wish to thank Prof. Elke Koch (Institute for Mineralogy, Petrology and Crystallography, University of Marburg) and Prof. Giovanni Ferraris (DSMP, University of Torino) for profitable discussions. Comments from an anonymous referee helped improving the clearness of the manuscript.

### References

Arakcheeva, A. V.; Chapuis, G.; Meyer, M.: The LT phase of $Cs_3Bi_2I_9$. Z. Kristallogr. **216** (2001) 199–205.

Buerger, M. J.: The Diffraction Symmetry of Twins. Anaias de Acad. Bras. de Ciéncias **26** (1954) 111–121 [later republished in Buerger, M. J.: X-Ray Crystallography, John Wiley & Sons, New York (1962) 53–67].

Curien, H.; Donnay, J. D. H.: The Symmetry of the Complete Twin. Am. Mineral. **44** (1959) 1067–1070.

Curien, H.; Le Corre, Y.: Notations des macles à l'aide du symbolisme des groupes de couleurs de Choubnikov. Bull. Soc. franç. Minér. Crist. **81** (1958) 126–132.

Donnay, G.; Donnay, J. D. H.: Classification of Triperiodic Twins. Can. Mineral. **12** (1974) 422–425.

Ferraris, G.; Gula, A.; Ivaldi, G.; Nespolo, M.; Raade, G.: Crystal structure of kristiansenite: a case of class IIB twinning by metric merohedry. Z. Kristallogr. **216** (2001) 442–448.

Friedel, G.: Étude sur les groupements cristallins. Extrait du *Bullettin de la Société de l'Industrie minérale*, Quatrième série, Tomes III et IV. Saint-Étienne, Societè de l'Imprimerie Thèolier J. Thomas et C., (1904) 485 pp.

Friedel, G.: Leçons de Cristallographie., Berger-Levrault, Nancy, Paris, Strasbourg (1926) XIX + 602 pp.

Friese, K.; Kienle, L.; Duppel, V.; Luo H.; Lin, C.: Single-crystal X-ray diffraction and electron-microscopy study of multiple-twinned $Sr_3(Ru_{0.336},Pt_{0.664})CuO_6$. Acta Crystallogr. **B59** (2003) 182–189.

Grimmer, H.: Determination of all misorientations of tetragonal lattices with low multiplicity; connection with Mallard's rule of twinning. Acta Crystallogr. **A59** (2003) 287–296.

Hahn, T.; Klapper, H.: Crystallographic and noncrystallographic point groups. Sect. **10** in Th. Hahn (Ed.) *International Tables for Crystallography*, Vol. A, 5th edition. International Union of Crystallography / D. Reidel Publishing Company (2002).

Hahn, T.; Klapper, H.: Twinning of crystals. Sect. **3.3** in A. Authier (Ed.) *International Tables for Crystallography*, Vol. D, edition. International Union of Crystallography/D. Reidel Publishing Company (2003).

Harker, D.: A Table of the Colored Crystallographic and Icosahedral Point Groups, Including Their Chirality and Diamorphism. Acta Crystallogr. **A32** (1976) 133–139.

Hartman, P.: On the Morphology of Growth Twins. Z. Kristallogr. **107** (1956) 225–237.

Henke, H.: Crystal structures, order-disorder transition and twinning of the Jahn-Teller system $(NO)_2VCl_6$. Z. Kristallogr. **218** (2003) 617–625.

Herbst-Irmer, R.; Scheldrick, G. M.: Refinement of Twinned Structures with *SHELXL97*. Acta Crystallogr. **B54** (1998) 443–449.

Le Corre, Y.: Les groupes de symétrie bicolores et leurs applications. Bull. Soc. franç. Minér. Crist. **81** (1958) 120–125.

Nespolo, M.; Ferraris, G.: Twinning by syngonic and metric merohedry. Analysis, classification and effects on the diffraction pattern. Z. Kristallogr. **215** (2000) 77–81.

Nespolo, M.; Ferraris, G.: Geminography – The science of twinning applied to the early-stage derivation of non-merohedric twin laws. Z. Kristallogr. **218** (2003) 178–181.

Nespolo, M.; Ferraris, G.: Applied Geminography – Symmetry analysis of twinned crystals and definition of twinning by reticular polyholohedry. Acta Crystallogr. A**60** (2004) 89–95.

Onoda, M.; Chen, X.-A.; Kato, K.; Sato, A.; Wada. H: Structure refinement of $Cu_8GeS_6$ using X-ray diffraction data from a multiple-twinned crystal. Acta Crystallogr. **B55** (1999) 721–725 (erratum: p. 1109).

Quarez, E.; Huve, M.; Roussel, P.; Mentré, O.: Polysynthetic twinning characterization and crystallographic refinement in $NaBa_2M_2^{2+}M^{3+}O_6$ ($M = Ni$, Cu). J. Solid St. Chem. **165** (2002) 214–227.

Sadanaga, R.; Sawada, T.; Ohsumi, K.; Kamiya, K.: Classification of superstructures by symmetry. J. Jpn. Assoc. Min. Petr. Econ. Geol. Spec. **2** (1980) 23–29.

Shafranovskii, I. I.; Pis'mennyi, V. A.: General forms of twinned structures. Sov. Phys. Cristallogr. **6** (1961) 27–33.

Shubnikov, A. V.; Koptsik, V. A.: Symmetry in Science and Art. New York, London: Plenum Press (1974) XXV + 420 pp.

Takano, Y.: Classification of twins. IV. Ordinary twins. J. Jpn. Assoc. Min. Petr. Econ. Geol. **67** (1972) 345–351.

Takano, Y.: Twin Point Groups. Tokyo: Kokon (1973) 127 pp. (in Japanese).

Vainshtein, B.: Fundamentals of Crystals. Corr. printing of the 2nd enlarged edition. Berlin: Springer (1996) XXI + 482 pp.

Van der Warden, B.; Burckhardt, J. J.: Farbgruppen. Z. Kristallogr. **115** (1961) 213–234.

Wittke, O.; Garrido, J.: Simétrie des polyhèdres polychromatiques. Bull. Soc. franç. Minér. Crist. **82** (1959) 223–230.

Zorkii, P. M.: The supersymmetry of molecular crystal structures. Acta Crystallogr. **A34** (1978) S1–S2.