$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$)+ appears. This means that the full set of displacements corresponding to a particular composite symmetry is obtained by adding the vector $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ in turn to all displacements of the set given in the first column. The full set of displacements contains all the vectors whose end-points are equivalent positions in the space group of the vector set associated with the original composite. Such a set of displacements will be referred to as 'set of equivalent displacements' and the number of equivalent displacements in the set is called its rank.

In part I we pointed out there are displacements which create symmetry-related composites. This is true for periodic composites as well. In this case, however, the periodicity of the spatial symmetry variation must also be taken into account. If the translational symmetry of the vector set of a periodic composite is described by a primitive lattice, then the set of equivalent displacements contains all the shift vectors which yield symmetry-related composites. On the other hand, for vector sets with non-primitive lattices the set of equivalent displacements contains in addition displacements which are associated with identical composites. This is the case for the above-considered example. The equivalent displacements $(0, 0, z)$, $(0, 0, \bar{z})$, $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}+z)$, $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}-z)$, for instance, yield composites with symmetry $I42'2'$. But all these composites are not symmetry equivalent. The first and third, as well as the second and fourth, displacements are interrelated by the translation vector $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ of the vector set and, hence, they correspond to identical composites. Thus, the number of symmetry-related composites depends on whether the lattice of the vector set (or, equivalently, of the periodic composite; see Buerger, 1959) is primitive or not. The number of symmetry-related composites is equal to the rank of the set of equivalent displacements divided by the number of lattice points in the unit cell of the periodic composite. This can be expressed comprehensively through a detailed study of the symmetry-related composites obtained by general and special displacements. Such a formulation in group theoretical terms will, however, be discussed in a following paper.

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Composite Symmetry Formed by Two Identical Point Groups With Common Origin

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Abstract

A group-theoretical method is presented that enables the derivation of the symmetry of any composite created by the superposition of two identical point groups. The invariant points of the two components are considered in coincidence and the composite symmetry is expressed as the intersection of two sets of symmetry operations. The first set contains the symmetry operations common in the components when their mutual disposition is taken into account, whereas in the second set belong the additional

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symmetry operations relating the two equivalent components. The existence of such symmetrizing operations is revealed particularly clearly by using the framework of two-coloured symmetry. Analytical expressions for the operations of each set are derived in terms of the mutual orientation of the two components and theorems are given for the determination of the composite point symmetry when the components are rotated relative to each other along a direction passing through their origin. The application of the methodology is demonstrated by considering particular examples and a table of all possible composite symmetry groups associated with superpositions of the 32 crystallographic point groups is given.

1. Introduction

In the study of the symmetry of composites we first note that they are characterized by a specific combination of two or more components. The symmetry of such complex systems depends on the number, symmetry, relative position and relative orientation of their parts. Thus, in order to express relations between the components and the whole we classify the composites into several categories. In this way, we are able to correlate the composite symmetry to, say, the number of components of certain symmetry and specific combination. Or, we can study the symmetry of a composite in relation to only the relative position and orientation of its components which are of given number and symmetry.

The composites considered in this paper consist of two identical finite components of crystallographic symmetry having their invariant points in coincidence. The symmetry of such composites depends only on the relative orientation and point symmetry of the components. In other words, we consider two identical point groups superposed so that they have common origin and we investigate the various types of point symmetry created as the component groups are rotated relative to each other along a direction passing through their origin.

This problem is of particular interest in the investigation of the symmetry of bicrystals. Pond & Bollmann (1979) proposed that a bicrystal can be considered, for the purpose of symmetry studies, as the composite created by the superposition of two semi-infinite crystals. Also, they pointed out that the point symmetry of the bicrystal can be determined by inspection of the configuration formed by two geometrical figures modelling the symmetry of the semi-infinite crystals. However, the relationship between composite point symmetry and relative rotation of the components can be investigated analytically by the group-theoretical approach presented in this paper.

2. Notation

In this work concepts from two-coloured symmetry are extensively used. The symbols of the two-coloured groups are constructed according to the Hermann–Mauguin extended scheme, the fundamentals of which are given by Koptsik (1966) and Shubnikov & Koptsik (1974). Colour-reversing symmetry elements, as well as colour-reversing symmetry operations, are designated by a 'prime' which implies that the corresponding ordinary element or operation is followed by colour exchange.

The symbols of the symmetry operations are given according to the scheme proposed by Donnay & Donnay (1972). Thus, the Hermann–Mauguin symbols that normally refer to symmetry axes also represent symmetry operations provided the power of the operation be explicitly stated. By convention the rotation of the symmetry axes (and, therefore, of the corresponding symmetry operations) is considered in the right-handed (anticlockwise) sense. As to the symmetry operations of inversion and reflection the letters i and s provide self-explanatory symbols.* Subscripts are used to indicate the direction of the symmetry element or operation; the same subscripts on m or s indicate the direction of the normal to the plane of reflection.

3. The geometrical interpretation of the Neumann–Curie principle

The basis of the proposed group-theoretical approach is the geometrical interpretation of the Neumann–Curie principle (see *e.g.* Shubnikov & Koptsik, 1974) outlined in this section. Consider the simple case of superposing the symmetries of a square and a rectangle where their geometrical centres and twofold symmetry axes coincide. The square (on a one-sided plane) has symmetry $G_1 = 4mm$ while the rectangle has symmetry $G_2 = 2mm$. If the planes of symmetry of the two figures coincide (Fig. 1*a*), then the composite as a whole possesses the symmetry of the highest common subgroup of these two groups, namely $G = 2mm$. It should be mentioned, however, that in determining the symmetry of a composite the mutual disposition of its components must be taken into account. This is shown in Fig. 1(*b*) where the two figures have now no common planes of symmetry and, hence, the highest common subgroup for the particular orientation is $G' = 2$ (*i.e.* the common twofold axis perpendicular to the plane of the figures).

The process of forming a composite from non-equivalent parts is accompanied by the 'dissymmetrization' of the system since it leads to a reduction in

* Note that the symmetry element of mirror reflection is represented by m and the mirror operation by s. This is, in fact, the only departure from the Hermann–Mauguin notation.

the symmetry of the whole in comparison with the symmetry of the parts. The opposite process, 'symmetrization', occurs on forming composites from equivalent parts. Fig. 1(c) shows a figure composed of two identical rectangles ($G_1 = G_2 = 2mm$) which have common centres and are rotated by 90° relative to each other. In this case the symmetry of the composite is $G = 4mm$. Thus, if the components are geometrically identical then the symmetry group of the composite may be a supergroup of the symmetry groups of the components.

As was mentioned above a necessary condition imposed by the Neumann–Curie principle is that the relative orientation of the components must be taken into account in order to determine the symmetry operations of the composite. An immediate consequence of this condition is illustrated in Fig. 1(c). After the superposition of the two rectangles the twofold axes of the separate components coincide and, hence, the composite has also a twofold symmetry axis. But when superposed there is further symmetry in the composite: any point of one component is related to a similar point of the other component by the rotation which relates the two parts. Therefore, the composite has the common symmetry of the individuals augmented by the operation of the rotation which describes their mutual orientation.

This example indicates that in the case of symmetrization the composite may contain symmetry elements created not by the coincidence but by the appropriate orientation of the symmetry elements of the components. The difference between the two kinds of symmetry operations present in a composite becomes straightforward if we introduce the concept of colour-reversing (or antisymmetry) operations. These are symmetry operations which transfer the object to a symmetrically related position and change its colour from white to black or *vice versa*. For employing this concept one of the components is designated 'white' and the other 'black'; this designation is, however, quite arbitrary and there is no difference between a white and a black point except that they belong to different components. Superposition of the white and black components creates a 'dichromatic composite' with symmetry generally different to that of the components. This is because (a) symmetry operations parallel to one another in both the white and black components are conserved as ordinary symmetry operations; and (b) symmetry operations of the components not parallel after the superposition are suppressed; yet they can give rise to colour-reversing operations in the composite.

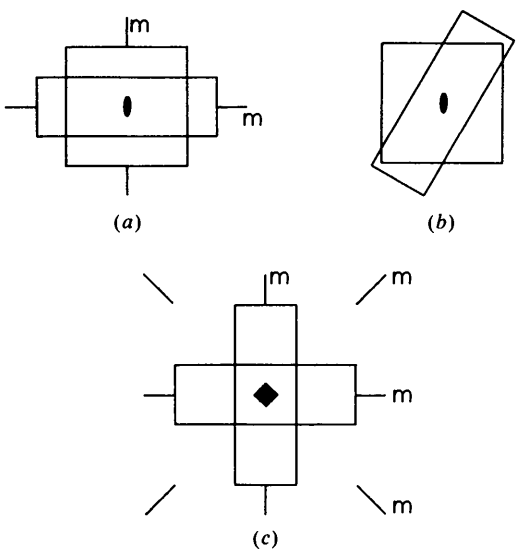

Fig. 1. Geometrical interpretation of the Neumann–Curie principle. The superposition of the point groups $4mm$ (square) and $2mm$ (rectangle) leads to a composite with symmetry either $2mm$ [when $4mm$ and $2mm$ have common mirror planes, (a)] or 2 (b). On the other hand, the superposition of the two rectangles in (c) corresponds to symmetrization and yields a composite with symmetry $4mm$.

4. Group-theoretical formulation of the superposition of point symmetries

In order to study the point symmetry of a dichromatic composite we consider its white component fixed in orientation and position so that it acts as the reference component. The dichromatic composite is then obtained by the operation $\{[xyz]/\theta\}'$, which means that a component originally coincident with the reference component and with the same colour is rotated by an angle θ about $[xyz]$ (using the white coordinate system) and subsequently undergoes colour reversal from white to black (as represented by the prime). The operation $\{[xyz]/\theta\}$ describes the misorientation (*i.e.* the misalignment between the two individuals of the composite) of the two components.

The following notation is now introduced. The point group of the white component is designated G_w with elements, expressed relative to the white coordinate system, g_i and of order r_w. Also, the point group of the black component, designated G_b, is of order $r_b = r_w$ and its elements, expressed relative to the black coordinate system, are identical to g_i, $i = 1,2,\ldots,r_w$.

After rotation $\{[xyz]/\theta\}'$ the two components are brought out of alignment and the black and white points are not in coincidence except the common origin. The symmetry operations of G_w are g_i, whereas those of G_b are expressed relative to the white coordinate system by $R'g_iR'^{-1}$, where R' is the matrix describing the vector transformation of the black component.* The composite obtained by $\{[xyz]/\theta\}'$ will, in general, contain ordinary and colour-reversing symmetry operations as explained below.

* R' is always a colour-reversing rotation. Bearing this in mind we shall write R instead of R'.

4.1. *Ordinary symmetry operations of the composite point group*

An ordinary symmetry operation describes, by definition, the relationship between points of the same colour. Thus, such an operation is present in the dichromatic composite only when it expresses a geometrical relationship which is satisfied by the set of white points as well as by the set of black points. In other words, this symmetry operation must be common for the white and black components since the rotation $\{[xyz]/\theta\}'$ changes only the misorientation of the components but does not alter the black or white configurations. Therefore, the necessary and sufficient condition for an ordinary symmetry operation to be present in the composite point group G_c is that, after rotation, identical elements of G_w and G_b are coincident. This implies, of course, that the elements of G_w and G_b are expressed relative to the same coordinate system which in our considerations is the system of the white component unless specifically stated to be otherwise. Consequently, the following theorem is self-evident.

Theorem 1: The ordinary symmetry operations in the dichromatic composite point group are the only elements of G_w which satisfy the relation $g_i = Rg_jR^{-1}$, where R is the matrix describing the vector transformation of the black component and g_i, g_j are expressed relative to the coordinate system of the white component.

Now, let D_0 be the set of elements of G_w satisfying the relation of theorem 1. We can prove the following theorem (the proofs of the theorems are given for clarity in the Appendix*).

Theorem 2: The ordinary symmetry operations of the composite point group form a subgroup (trivial or not) of the point group of the white component.

The elements of the group D_0 are denoted by h_i, and they satisfy the relation

$$h_i = Rh_jR^{-1}. \quad (1)$$

Theorem 2 immediately yields (see Appendix) the following.

Theorem 3: The order of the composite point group, r, is equal to $2/\kappa$ times the order of the point group G_w, where κ is a positive integer.

A consequence of the last theorem is that only symmetry operations of order equal to or less than twice the order of the point group G_w are present in a composite point group. The equality, however, holds only when the composite point group is a cyclic group. Also, as was mentioned in the proof of theorem 3, the order of the composite point group is always twice the order of D_0. Now, since D_0 is a subgroup of G_w, the lowest and highest orders of D_0 correspond to the trivial subgroups of G_w. Therefore, we have the following.

Theorem 4: The lowest order of the composite point group is 2 and the highest is $2r_w$, where r_w is the order of the white point group.

A dichromatic composite with the lowest possible symmetry can be created by the exact superposition of two point groups with symmetry $G_w = G_b = 1$. In this case the composite point group is $G_c = 11'$ (grey point group). More interesting, however, is the case of a composite with the highest symmetry $r = 2r_w$. Such a case corresponds to the process of symmetrization and a particular example is shown in Fig. 1(*c*) where $G_w = G_b = 2mm$ with order $r_w = 4$. Thus, if the components are regarded as white and black, the appropriate orientation of the two superposed figures results in a composite with symmetry $G_c = 4'mm'$ of order $r = 2r_w = 8$.

4.2. *Colour-reversing symmetry operations of the composite point group*

Our attention is now focused on the colour-reversing symmetry operations of the composite point group. We need to find an expression describing the colour-reversing transformations which may be present in the composite of arbitrary misorientation and, then, we must determine the conditions under which these transformations, together with the ordinary operations given by theorem 1, form a group. We start by noting that the composite point group contains two sets of general points which, according to the discussion in the foregoing section, are

white points: $\{h_1\mathbf{w}, h_2\mathbf{w}, \ldots, h_{r_0}\mathbf{w}\}$
black points: $\{h_1\mathbf{b}, h_2\mathbf{b}, \ldots, h_{r_0}\mathbf{b}\}$,

where **w** and **b** are the white and black 'starting' points respectively, and h_i ($i = 1,2,\ldots, r_0$, where r_0 is the order of D_0) are the elements of the group D_0. The relationship between the vectors **w** and **b** can be determined if it is borne in mind that the black points are obtained by a rotation of the white ones. Thus, $\mathbf{b} = Rg_k\mathbf{w}$, where g_k is a symmetry operation of G_w; g_k may or may not be an element of D_0. Therefore, the above sets of points can be written as

white points: $\{h_1\mathbf{w}, h_2\mathbf{w}, \ldots, h_{r_0}\mathbf{w}\}$
black points: $\{h_1Rg_k\mathbf{w}, h_2Rg_k\mathbf{w}, \ldots, h_{r_0}Rg_k\mathbf{w}\}$.

Any colour-reversing symmetry element of the composite point group must relate, by definition, at least a white and a black point of the above sets to each other. Consequently, the colour-reversing transformations c_m are given by $c_m = h_ig_k^{-1}R^{-1}h_j^{-1}$. But, since $h_j^{-1} \in D_0$ there is an element $h_n \in D_0$ such that h_j^{-1} and h_n satisfy (1): $h_j^{-1} = Rh_nR^{-1}$. Thus, replacing

* The Appendix, giving proofs of theorems 2, 3, 5 and 6, has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 38933 (5 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

h_j^{-1} by Rh_nR^{-1} we have $c_m = h_i g_k^{-1} h_n R^{-1}$, or

$$c_m = h_i g_m h_n R^{-1} \qquad (2)$$

where g_m is the reverse element of g_k in G_w. As was mentioned above, g_k, and therefore $g_m \equiv g_k^{-1}$, may or may not belong to D_0. Thus, we must consider two cases:

(i) $g_m \in D_0$, *i.e.* $g_m \equiv h_m$: then the colour-reversing transformations are given by

$$c_i = h_i R^{-1} \qquad (3a)$$

with h_i an element of D_0, and

(ii) $g_m \notin D_0$: taking $g_m h_n = h_q g_p$ we can express (2) in the form $c_m = h_i h_q g_p R^{-1}$, or

$$c_j = g_j R^{-1} \qquad (3b)$$

where g_j belongs to G_w but not to D_0 (*i.e.* g_m belongs to the set $G_w - D_0$).

However, not all transformations of the type (3*a*) or (3*b*) may occur as symmetry operations of the composite point group. Relations (3*a*) and (3*b*) lead, though, to an algorithm, as yet incomplete, for finding the point group of a composite formed by two components in given misorientation R. We consider the point group G_w of the components and we take its subgroups $D_{0,i}$ in sequence of decreasing order. For each $D_{0,i}$ which is invariant by the rotation R we form the products $c_i = h_i R^{-1}$ and $c_j = g_j R^{-1}$. If the set of elements h_i and $h_i R^{-1}$ or h_i and $g_j R^{-1}$ forms a group, then this is the required composite point group associated with the subgroup $D_{0,i}$. This algorithm would allow us to derive the point symmetry of the dichromatic composite obtained by the given misorientation R. However, the determination of the composite point group by means of the proposed algorithm is extremely laborious, since it involves checking the group property for many sets of elements.

In order to perfect an algorithm we prove the following theorems which make it easier to pick out rotations for which a composite point group is automatically formed. For this, we investigate the conditions under which the colour-reversing transformations given by (3*a*) or (3*b*) are indeed symmetry operations of the composite point group. The set of the colour-reversing transformations c_m is denoted by D_c and we require that the set of transformations $D = D_0 + D_c$ is a group in the mathematical sense of the word (the summation is to be understood as a juxtaposition of elements).

4.2.(*a*) *Case* I ($c_m = h_m R^{-1}$). According to (3*a*) the colour-reversing transformations are given by $c_m = h_m R^{-1}$, where h_m belongs to D_0, and the rotation yielding a composite point group is determined by the following (Appendix).

Theorem 5: The set $D = D_0 + D_c = \{h_1, h_2, \ldots, h_{r_0}, h_1R^{-1}, h_2R^{-1}, \ldots, h_{r_0}R^{-1}\}$ is a group if the rotation R satisfies the relation $R^2 = h_\alpha$, where h_α is a given element of D_0, and leaves the subgroup D_0 of G_w invariant.

4.2.(*b*) *Case* II ($c_m = g_m R^{-1}$). In the case of (3*b*) the colour-reversing transformations are given by $c_m = g_m R^{-1}$ with g_m belonging to $G_w - D_0$. This means that in this case the set D is associated not only with the elements h_i of D_0 but also with r_0 elements g_m of $G_w - D_0$. Now, we introduce the symbol D_2 for the set containing all the operations of the white point group G_w which are included (either as ordinary operations or in colour-reversing transformations through the relation $c_m = g_m R^{-1}$) in the set D, *i.e.* $D_2 = \{h_1, h_2, \ldots, h_{r_0}, g_1, g_2, \ldots, g_{r_0}\}$. The elements of the set $D_2 - D_0$ are denoted by f_i, $i = 1,2,\ldots, r_0$ so that $D_2 = \{h_1, h_2, \ldots h_{r_0}, f_1, f_2, \ldots, f_{r_0}\}$ with f_i belonging to $G_w - D_0$. We have the following (Appendix).

Theorem 6: The set $D = \{h_1, h_2, \ldots, h_{r_0}, f_1R^{-1}, f_2R^{-1}, \ldots, f_{r_0}R^{-1}\}$ is a group if: (*a*) D_2 is a factor 2 supergroup of D_0 and at the same time a subgroup of G_w, (*b*) the rotation R leaves D_0 invariant, and (*c*) the rotation R satisfies the relation $f_\alpha R^{-1} f_\alpha R^{-1} = h_\beta$, where h_β is an element of D_0 and f_α an element of $G_w - D_0$ such that $f_i = h_i f_\alpha$ for any f_i of $D_2 - D_0$.

5. Algorithm for the determination of composite point groups

Now we can formulate the final algorithm for finding the point symmetry of a dichromatic composite obtained by the superposition of two identical point groups with common origin. Two cases are to be considered: (1) R is a given rotation; and (2) R is any rotation, in which case we seek the distinct composite point groups corresponding to different misorientations of the two components.

(1) According to theorem 1, the ordinary symmetry operations of the composite point group are these elements of G_w which are invariant with respect to the rotation R. Thus, we form products of the type RgR^{-1} and allow g to be in turn each of the elements of the group G_w. The elements g_i for which Rg_iR^{-1} belongs to G_w will make up the group D_0. Next, we examine the form of the rotation R. If R^2 equals an element of D_0, then the composite point group is, according to theorem 5, $D = D_0 + D_0R^{-1}$. Otherwise, we take all subgroups of G_w which are index 2 supergroups of D_0; we denote them $D_{2,i}$ with elements f_{ij}, $j = 1,2,\ldots, r_0$. For each $D_{2,i}$ we form the product $f_{ij}R^{-1}f_{ij}R^{-1}$ with f_{ij} an element of $D_{2,i}$. If $f_{ij}R^{-1}f_{ij}R^{-1}$ belongs to D_0 then the composite point group is, according to theorem 6, $D = D_0 + D_0 f_{ij} R^{-1}$.

(2) In the second case R is not fixed but it varies over the range of permissible misorientation relationships of the two identical point groups, and we want

Table 1. *Determination of the composite point group formed by the superposition of two cubic point groups m3m with misorientation* {[001]/45°}

g_i	Rg_iR^{-1}	h_iR^{-1}	g_i	Rg_iR^{-1}	h_iR^{-1}	g_i	Rg_iR^{-1}	h_iR^{-1}	g_i	Rg_iR^{-1}	h_iR^{-1}
1	1	$8^{1'}_{001}$	$2^1_{\bar{1}01}$			i	i	$\bar{8}^{1'}_{001}$	$s_{\bar{1}01}$		
$3^1_{1\bar{1}1}$			2^1_{011}			$\bar{3}^1_{1\bar{1}1}$			s_{011}		
$3^2_{1\bar{1}1}$			$2^1_{0\bar{1}1}$			$\bar{3}^5_{1\bar{1}1}$			$s_{0\bar{1}1}$		
3^1_{111}			4^1_{001}	4^1_{001}	$8^{3'}_{001}$	$\bar{3}^1_{111}$			$\bar{4}^1_{001}$	$\bar{4}^1_{001}$	$\bar{8}^{7'}_{001}$
3^2_{111}			4^3_{001}	4^3_{001}	$8^{7'}_{001}$	$\bar{3}^5_{111}$			$\bar{4}^3_{001}$	$\bar{4}^3_{001}$	$\bar{8}^{3'}_{001}$
$3^1_{\bar{1}11}$			4^1_{010}			$\bar{3}^1_{\bar{1}11}$			$\bar{4}^1_{010}$		
$3^2_{\bar{1}11}$			4^3_{010}			$\bar{3}^5_{\bar{1}11}$			$\bar{4}^3_{010}$		
$3^1_{\bar{1}\bar{1}1}$			4^1_{100}			$\bar{3}^1_{\bar{1}\bar{1}1}$			$\bar{4}^1_{100}$		
$3^2_{\bar{1}\bar{1}1}$			4^3_{100}			$\bar{3}^5_{\bar{1}\bar{1}1}$			$\bar{4}^3_{100}$		
2^1_{110}	2^1_{100}	$2^{1'}_{\nu}$	2^1_{100}	$2^1_{\bar{1}10}$	$2^{1'}_{\tau}$	s_{110}	s_{100}	s'_{ν}	s_{100}	$s_{\bar{1}10}$	s'_{τ}
$2^1_{\bar{1}10}$	2^1_{010}	$2^{1'}_{\rho}$	2^1_{010}	2^1_{110}	$2^{1'}_{\xi}$	$s_{\bar{1}10}$	s_{010}	s'_{ρ}	s_{010}	s_{110}	s'_{ξ}
2^1_{101}			2^1_{001}	2^1_{001}	$8^{5'}_{001}$	s_{101}			s_{001}	s_{001}	$\bar{8}^{5'}_{001}$

Note: The subscripts ρ, τ, ν, ξ correspond to the directions $[\sqrt{2+\sqrt{2}}, \sqrt{2-\sqrt{2}},0]$, $[\sqrt{2-\sqrt{2}}, \sqrt{2+\sqrt{2}},0]$, $[-\sqrt{2-\sqrt{2}}, \sqrt{2+\sqrt{2}},0]$, $[-\sqrt{2+\sqrt{2}}, \sqrt{2-\sqrt{2}},0]$, respectively. These directions have an angular distance of 22·5° in the anticlockwise sense from the directions [100], [110], [010], and [$\bar{1}$10], respectively.

to determine the distinct composite point groups obtained. This is achieved by the following procedure. We start by taking the list of subgroups (trivial or not) of the given point group G_w. For each subgroup D_0 rotations can be found leading to at least one composite point group. Such rotations are determined according to either theorem 5 or theorem 6.

We consider first the case where the colour-reversing transformations are given by $c_i = h_iR^{-1}$ with h_i belonging to D_0. The composite point groups corresponding to D_0 are then determined by taking separately each element of D_0 and applying theorem 5. Thus, for each subgroup $D_{0,i}$ and each $h_j \in D_{0,i}$ we obtain a set of rotations R_k such that (*a*) $R_k^2 = h_j$ and (*b*) $R_kD_{0,i}R_k^{-1} = D_{0,i}$ (*i.e.* $D_{0,i}$ is invariant with respect to R_k). For any such rotation R_k the composite point group has the form $D = D_{0,i} + D_{0,i}R_k^{-1}$.

Finally, there remains the consideration of the case of composite groups with colour-reversing operations of the type $c_i = f_iR^{-1}$. According to theorem 6 a composite group $D = D_0 + D_0f_iR^{-1}$, with $f_i \in D_2 - D_0$, is formed for rotations R such that $f_iR^{-1}f_iR^{-1} \in D_0$. We note, however, that if we substitute $R_1^{-1} = f_iR^{-1}$ then this case is reduced to the one mentioned just above. Thus, in order to determine the rotations yielding composite groups of the form $D = D_0 + D_0f_iR^{-1}$ we work as follows. We consider each composite group $D = D_0 + D_0R_\alpha^{-1}$ separately and we take the index 2 extensions of D_0: $D_2 = D_0 + D_0f_i$. For each such extension belonging to G_w a composite point group $D = D_0 + D_0f_iR^{-1}$, isomorphous to $D = D_0 + D_0R_\alpha^{-1}$, will correspond to the rotation $R^{-1} = f_i^{-1}R_\alpha^{-1} = (R_\alpha f_i)^{-1}$.

6. Application of the algorithm

We consider now two examples for demonstrating the application of the proposed algorithm. In the first example the point group of the two components is the cubic group $G_w = m3m$ and the misorientation of the components is described by the rotation {[001]/45°}'. The reference coordinate system is orthogonal and has the standard setting (*International Tables for X-ray Crystallography*, 1965) with respect to the white point group. The group G_w contains 48 elements given in Table 1 under the heading g_i. The ordinary symmetry elements of the dichromatic composite are those elements of G_w for which Rg_iR^{-1} belongs to G_w with

$$R = \begin{pmatrix} \sqrt{2}/2 & -\sqrt{2}/2 & 0 \\ \sqrt{2}/2 & \sqrt{2}/2 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Thus, according to the second column of Table 1, we have $D_0 = 4/mmm$. The rotation R satisfies the equation $R^2 = 4^1_{001}$ and, therefore, the composite point group is of the form $D = D_0 + D_0R^{-1}$. The colour-reversing elements of this group are given in the column h_iR^{-1} in Table 1. We note that in the dichromatic composite there is an eightfold colour-reversing axis (*i.e.* the set of symmetry operations $1, 8^{1'}_{001}, 4^1_{001}, 8^{3'}_{001}, 2^1_{001}, 2^1_{001}, 8^{5'}_{001}, 4^3_{001}, 8^{7'}_{001}$) and according to the tables given by Vlachavas (1980) (see also Vlachavas, 1984; following paper) the composite point group is $8'/mm'm'$. This example illustrates the possibility of non-crystallographic composite point groups (see below).

In the second example considered here we determine the distinct composite groups corresponding to $G_w = 222 = \{1, 2^1_{100}, 2^1_{010}, 2^1_{001}\}$. Its subgroups are $D_{0,1} \equiv G_w$, $D_{0,2} = \{1, 2^1_{100}\}$, $D_{0,3} = \{1, 2^1_{010}\}$, $D_{0,4} = \{1, 2^1_{001}\}$, $D_{0,5} = \{1\}$. For $D_{0,1}$ and $h_\alpha = 1$, the relation $R^2 = 1$ is satisfied for a proper or improper rotation of the form {[xyz]/360°}' or {[xyz]/180°}'. The former corresponds to either the anti-identity operation $1'$ or the anti-inversion operation $\bar{1}'$ and we note that both leave $D_{0,1}$ invariant. Thus, we have $D = D_{0,1} + D_{0,1}1' = 2221'$ and $D = D_{0,1} + D_{0,1}\bar{1}' = m'm'm'$ correspondingly.

The rotation $\{[xyz]/180°\}'$, on the other hand, corresponds to either a twofold colour-reversing operation along $[xyz]$ or a colour-reversing reflection perpendicular to $[xyz]$, and they leave $D_{0,1}$ invariant only when $[xyz]$ is along special directions. Thus, the operation $\{[xyz]/180°\}'$ will lead to a composite point group $D = D_{0,1} + D_{0,1}R^{-1}$ only when the rotation axis is parallel to any of the directions [100], [010], [001], [110], [$\bar{1}$10], [101], [$\bar{1}$01], [011], [0$\bar{1}$1] (or their opposites). We note, however, that the proper or improper rotation $\{[100]/180°\}'$ can be expressed as $2^1_{100}1'$ or $s_{100}1'$, respectively. Consequently, these rotations will yield

$$D = D_{0,1} + D_{0,1}2^1_{100}1' = D_{0,1} + D_{0,1}1' = 2221'$$

or

$$D = D_{0,1} + D_{0,1}s_{100}1' = D_{0,1} + \{s_{100}, i, s_{010}, s_{001}\}1'$$
$$= m'm'm'$$

(and similarly for $\{[010]/180°\}'$ and $\{[001]/180°\}'$).

Rotation $\{[110]/180°\}'$ corresponds to $2^{1'}_{110}$ or s'_{110} and, thus, it gives

$$D = D_{0,1} + D_{0,1}2^{1'}_{110} = D_{0,1} + \{2^{1'}_{110}, 4^{1'}_{001}, 4^{3'}_{001}, 2^{1'}_{\bar{1}10}\}$$
$$= 4'22'$$

or

$$D = D_{0,1} + D_{0,1}s'_{110} = D_{0,1} + \{s'_{110}, \bar{4}^{1'}_{001}, \bar{4}^{3'}_{001}, s'_{\bar{1}10}\}$$
$$= \bar{4}'2m'$$

(and similarly for one the proper and improper rotations along the rest of the directions mentioned above).

We turn our attention, now, to the second element of $D_{0,1}$, *i.e.* $h_\alpha = 2^1_{100}$, and the relation $R^2 = 2^1_{100}$ gives $R = \{[100]/90°\}'$ (and $\{[100]/270°\}'$). We can express R as $4^{1'}_{100}$ (and $4^{3'}_{100}$) or $\bar{4}^{3'}_{100}$ (and $\bar{4}^{1'}_{100}$) and we obtain

$$D = D_{0,1} + D_{0,1}4^{1'}_{100} = D_{0,1} + \{4^{1'}_{100}, 4^{3'}_{100}, 2^{1'}_{011}, 2^{1'}_{0\bar{1}1}\}$$
$$= D_{0,1} + D_{0,1}4^{3'}_{100} = 4'22'$$

or

$$D = D_{0,1} + D_{0,1}\bar{4}^{3'}_{100} = D_{0,1} + \{\bar{4}^{3'}_{100}, \bar{4}^{1'}_{100}, s'_{011}, s'_{0\bar{1}1}\}$$
$$= D_{0,1} + D_{0,1}\bar{4}^{1'}_{100} = \bar{4}'2m'.$$

Similarly, the remaining elements of $D_{0,1}$, *i.e.* 2^1_{010} and 2^1_{001}, will yield the composite point groups $4'22'$ (for the proper rotations $\{[010]/\pm 90°\}'$ and $\{[001]/\pm 90°\}'$) and $\bar{4}'2m'$ (for the corresponding improper rotations).

Next, we have to consider the subgroups $D_{0,2}$, $D_{0,3}$, $D_{0,4}$. However, we determine only the composite point groups associated with $D_{0,2}$, and we note that the algorithm can be applied identically for $D_{0,3}$ and $D_{0,4}$. For $D_{0,2} = \{1, 2^1_{100}\}$ and $h_\alpha = 1$ we have that R must be $\{[xyz]/360°\}'$, $\{[100]/180°\}'$ or $\{[0yz]/180°\}'$. The first two rotations have already been considered above and, thus, we have to examine only $\{[0yz]/180°\}'$ here. This rotation may be proper or improper, expressed as $2^{1'}_{0yz}$ or s'_{0yz}, respectively. The composite point groups obtained are

$$D = D_{0,2} + D_{0,2}2^{1'}_{0yz} = \{1, 2^1_{100}, 2^{1'}_{0yz}, 2^{1'}_{0\bar{z}y}\} = 22'2'$$

or

$$D = D_{0,2} + D_{0,2}s'_{0yz} = \{1, 2^1_{100}, s'_{0yz}, s'_{0\bar{z}y}\} = 2m'm'.$$

For the subgroups $D_{0,3}$ and $D_{0,4}$ the groups $22'2'$ and $2m'm'$ are obtained by the rotations $\{[x0z]/180°\}$ and $\{[xy0]/180°\}'$, respectively. For $D_{0,2} = \{1, 2^1_{100}\}$ and $h_\alpha = 2^1_{100}$ we have R is $\{[100]/90°\}'$, which, however, has already been considered above.

The remaining subgroup $D_{0,5} = \{1\}$ will yield two rotations: $\{[xyz]/360°\}'$ (already considered above) or $\{[xyz]/180°\}'$. The latter corresponds to $2^{1'}_{xyz}$ or s'_{xyz} and, thus, $D = D_{0,5} + D_{0,5}2^{1'}_{xyz} = \{1, 2^{1'}_{xyz}\} = 2'$ or $D = D_{0,5} + D_{0,5}s'_{xyz} = \{1, s'_{xyz}\} = m'$, respectively.

Finally, we determine the rotations corresponding to theorem 6. Let the composite point group $22'2' = \{1, 2^1_{001}, 2^{1'}_{x0z}, 2^{1'}_{\bar{z}0x}\} = D_{0,4} + D_{0,4}R^{-1}$, where R is the proper rotation $\{[xy0]/180°\}'$. The point group $G_w = 222$ can be written as $222 = D_{0,4} + D_{0,4}2^1_{100} = D_{0,4} + D_{0,4}2^1_{010}$. Thus, the composite group $22'2'$ can be obtained not only by $\{[xy0]/180°\}'$ but also by $\{[xy0]/180°\}'2^1_{100}$ and $\{[xy0]/180°\}'2^1_{010}$. Now, the direction cosines of $[xyz]$ are $c_1 = \cos\theta_1$, $c_2 = \sin\theta_1$ and $c_3 = 0$ where θ is the angle between [100] and $[xy0]$, and the rotation $\{[xy0]/180°\}$ can be expressed as (Jeffreys & Jeffreys, 1950)

$$R = \begin{pmatrix} 2c_1^2 - 1 & 2c_1c_2 & 0 \\ 2c_1c_2 & 2c_2^2 - 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$
$$= \begin{pmatrix} \cos(2\theta_1) & \sin(2\theta_1) & 0 \\ \sin(2\theta_1) & -\cos(2\theta_1) & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

The rotation $\{[xy0]/180°\}'2^1_{100}$ is, therefore, written as

$$\begin{pmatrix} \cos(2\theta_1) & \sin(2\theta_1) & 0 \\ \sin(2\theta_1) & -\cos(2\theta_1) & 0 \\ 0 & 0 & -1 \end{pmatrix}\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$
$$= \begin{pmatrix} \cos(2\theta_1) & -\sin(2\theta_1) & 0 \\ \sin(2\theta_1) & \cos(2\theta_1) & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

or $\{[xy0]/180°\}'2^1_{100} = \{[001]/2\theta_1\}'$. Similarly, we have $\{[xy0]/180°\}'2^1_{010} = \{[001]/180° + 2\theta_1\}'$. Consequently, the composite point group $22'2' = \{1, 2^1_{001}, 2^{1'}_{x0z}, 2^{1'}_{\bar{z}0x}\}$ is obtained by one of the proper rotations $\{[xy0]/180°\}'$, $\{[001]/2\theta_1\}'$ and $\{[001]/180° + 2\theta_1\}'$. Table 2 summarizes the determination of the rotations corresponding to theorem 6 for the white group $G_w = 222$. The first column of this table gives the composite

Table 2. *Determination of the rotations corresponding to theorem 6 for the superposition of two point groups 222*

$\theta_1, \theta_2, \theta_3$ are the angles between [100] and the directions [$xy0$], [$x0z$] and [$0yz$], respectively.

$D = D_0 + D_0R^{-1}$ $D = D_0 + D_0(Rf_i)^{-1}$	R	D_0	$D_2 = D_0 + D_0f_i$	$R_1 = Rf_i$
$22'2' = \{1, 2^1_{001}, 2^{1'}_{xy0}, 2^{1'}_{\bar{y}x0}\}$	$\{[xy0]/180°\}'$	$\{1, 2^1_{001}\}$	$222 = D_0 + D_0 2^1_{100}$	$\{[001]/2\theta_1\}'$
			$222 = D_0 + D_0 2^1_{010}$	$\{[001]/180° + 2\theta_1\}'$
$2m'm' = \{1, 2^1_{001}, s'_{xy0}, s'_{\bar{y}x0}\}$	$\{[xy0]/180°\}'\bar{1}$	$\{1, 2^1_{001}\}$	$222 = D_0 + D_0 2^1_{100}$	$\{[001]/2\theta_1\}'\bar{1}$
			$222 = D_0 + D_0 2^1_{010}$	$\{[001]/180° + 2\theta_1\}'\bar{1}$
$22'2' = \{1, 2^1_{010}, 2^{1'}_{x0z}, 2^{1'}_{\bar{z}0x}\}$	$\{[x0z]/180°\}'$	$\{1, 2^1_{010}\}$	$222 = D_0 + D_0 2^1_{100}$	$\{[010]/2\theta_2\}'$
			$222 = D_0 + D_0 2^1_{001}$	$\{[010]/180° + 2\theta_2\}'$
$2m'm' = \{1, 2^1_{010}, s'_{x0z}, s'_{\bar{z}0x}\}$	$\{[x0z]/180°\}'\bar{1}$	$\{1, 2^1_{010}\}$	$222 = D_0 + D_0 2^1_{100}$	$\{[010]/2\theta_2\}'\bar{1}$
			$222 = D_0 + D_0 2^1_{001}$	$\{[010]/180° + 2\theta_2\}'\bar{1}$
$22'2' = \{1, 2^1_{100}, 2^{1'}_{0yz}, 2^{1'}_{0\bar{z}y}\}$	$\{[0yz]/180°\}'$	$\{1, 2^1_{100}\}$	$222 = D_0 + D_0 2^1_{010}$	$\{[100]/2\theta_3\}'$
			$222 = D_0 + D_0 2^1_{001}$	$\{[100]/180° + 2\theta_3\}'$
$2m'm' = \{1, 2^1_{100}, s'_{0yz}, s'_{0\bar{z}y}\}$	$\{[0yz]/180°\}'\bar{1}$	$\{1, 2^1_{100}\}$	$222 = D_0 + D_0 2^1_{010}$	$\{[100]/2\theta_3\}'\bar{1}$
			$222 = D_0 + D_0 2^1_{001}$	$\{[100]/180° + 2\theta_3\}'\bar{1}$

Table 3. *Antisymmetry point groups formed by the superposition of two identical point groups with common origin*

Point group of components	Antisymmetry point group of composite
1	$11'$ $\bar{1}'$ $2'$ m'
$\bar{1}$	$\bar{1}1'$ $2'/m'$
2	$21'$ $2/m'$ $22'2'$ $2m'm'$ $4'$ $\bar{4}'$ $2'$ m'
m	$m1'$ $2'/m$ $2'mm'$ $2'$ m'
$2/m$	$2/m1'$ $mm'm'$ $4'/m$ $2'/m'$
222	$2221'$ $m'm'm'$ $4'22'$ $\bar{4}'2m'$ $22'2'$ $2m'm'$ $2'$ m'
$2mm$	$2mm1'$ mmm' $4'mm'$ $\bar{4}'2'm$ $22'2'$ $2m'm'$ $2'mm'$ $2'$ m'
mmm	$mmm1'$ $4'/mmm'$ $mm'm'$ $2'/m'$
4	$41'$ $4/m'$ $42'2'$ $4m'm'$ $8'$ $\bar{8}'$ $2'$ m'
$\bar{4}$	$\bar{4}1'$ $4'/m'$ $\bar{4}2'm'$ $2'$ m'
$4/m$	$4/m1'$ $4/mm'm'$ $8'/m$ $2'/m'$
422	$4221'$ $4/m'm'm'$ $8'22'$ $\bar{8}'2m'$ $42'2'$ $4'22'$ $4m'm'$ $\bar{4}'2m'$ $22'2'$ $2m'm'$ $2'$ m'
$4mm$	$4mm1'$ $4/m'mm$ $8'mm'$ $\bar{8}'2'm$ $42'2'$ $4m'm'$ $2'mm'$ $2'$ m'
$\bar{4}2m$	$\bar{4}2m1'$ $4'/m'mm'$ $4'22'$ $\bar{4}'2m'$ $\bar{4}2'm'$ $22'2'$ $2m'm'$ $2'mm'$ $2'$ m'
$4/mmm$	$4/mmm1'$ $8'/mmm'$ $4'/mmm'$ $4/mm'm'$ $mm'm'$ $2'/m'$
3	$31'$ $\bar{3}'$ $32'$ $3m'$ $6'$ $\bar{6}'$ $2'$ m'
$\bar{3}$	$\bar{3}1'$ $\bar{3}m'$ $6'/m'$ $2'/m'$
32	$321'$ $\bar{3}'m'$ $6'22'$ $\bar{6}'2m'$ $32'$ $3m'$ $22'2'$ $2m'm'$ $4'$ $\bar{4}'$ $2'$ m'
$3m$	$3m1'$ $\bar{3}'m$ $6'mm'$ $\bar{6}'2'm$ $32'$ $3m'$ $2'mm'$ $2'$ m'
$\bar{3}m$	$\bar{3}m1'$ $6'/m'mm'$ $\bar{3}m'$ $4'/m$ $2'/m'$ $mm'm'$
6	$61'$ $6/m'$ $62'2'$ $6m'm'$ $\underline{12}'$ $\overline{\underline{12}}'$ $2'$ m'
$\bar{6}$	$\bar{6}1'$ $6'/m'$ $\bar{6}2'm'$ $2'$ m'
$6/m$	$6/m1'$ $6/mm'm'$ $\underline{12}'/m$ $2'/m'$
622	$6221'$ $6/m'm'm'$ $\underline{12}'22'$ $\overline{\underline{12}}'2m'$ $62'2'$ $6m'm'$ $4'22'$ $\bar{4}'2m'$ $22'2'$ $2m'm'$ $2'$ m'
$6mm$	$6mm1'$ $6/m'mm$ $\underline{12}'mm'$ $\overline{\underline{12}}'2'm$ $62'2'$ $6m'm'$ $2'mm'$ $2'$ m'
$\bar{6}m2$	$\bar{6}m21'$ $6'/mmm'$ $\bar{6}2'm'$ $4'mm'$ $\bar{4}'2'm$ $22'2'$ $2m'm'$ $2'mm'$ $2'$ m'
$6/mmm$	$6/mmm1'$ $\underline{12}'/mmm'$ $6/mm'm'$ $4'/mmm'$ $mm'm'$ $2'/m'$
23	$231'$ $m'3'$ $\bar{4}'3m'$ $4'32'$ $32'$ $3m'$ $6'$ $\bar{6}'$ $22'2'$ $2m'm'$ $2'$ m'
$m3$	$m31'$ $m3m'$ $\bar{3}m'$ $6'/m'$ $mm'm'$ $2'/m'$
432	$4321'$ $m'3'm'$ $8'22'$ $\bar{8}'2m'$ $6'22'$ $\bar{6}'2m'$ $4'22'$ $42'2'$ $4m'm'$ $\bar{4}'2m'$ $32'$ $3m'$ $22'2'$ $2m'm'$ $2'$ m'
$\bar{4}3m$	$\bar{4}3m1'$ $m'3'm$ $6'mm'$ $\bar{6}'2'm$ $\bar{4}2'm'$ $32'$ $3m'$ $2'mm'$ $2'$ m'
$m3m$	$m3m1'$ $8'/mmm'$ $6'/m'mm'$ $4'/mmm'$ $4/mm'm'$ $\bar{3}m'$ $mm'm'$ $2'/m'$

point groups as were determined above. We must notice that the maximum-order subgroup of G_w is not included in Table 2, since, according to theorem 6, this subgroup cannot yield a composite group of the form $D = D_0 + D_0f_iR^{-1}$. Also, the trivial subgroup $D_{0,5} = \{1\}$ does not appear in Table 2. This is because the composite groups associated with $D_{0,5}$ and derived according to theorem 5 correspond to rotations of general form. Consequently, any further investigation of these rotations would not be of any significance. The second and third columns of Table 2 give the rotation R and the subgroup D_0 associated with each composite group. In the next column the index 2 extensions of D_0 belonging to group 222 are shown. For any such extension the distinct rotations $R_1 = Rf_i$ yielding the particular composite group are given in the last column of Table 2.

7. Conclusions

The application of the algorithm was demonstrated for particular examples in the foregoing section. The superposition of any two identical point groups can be treated in a similar way. Table 3 gives the antisymmetry groups created by the superposition of a white and a black point group of crystallographic symmetry.

A number of interesting conclusions can be obtained from the application of the proposed algorithm. These are expressed in the following rules.

Rule 1: Rotations R being isomorphic to a symmetry operation of the white point group G_w yield a dichromatic composite with symmetry described by the grey point group $D=G_w+G_w1'$, where $1'$ is the anti-identity operation.

Let $R=g_\alpha 1'=1'g_\alpha$, then the relation $Rg_iR^{-1}=g_j$ becomes $g_\alpha 1'g_i1'g_\alpha^{-1}=1'g_\alpha g_ig_\alpha^{-1}1'=g_j$ and, thus, it holds for all the elements of the white point group. Also, $R^2=g_\alpha 1'g_\alpha 1'=g_\alpha^2\in G_w$. Consequently, this case corresponds to complete coincidence of the white and black point groups and, hence, the dichromatic point group is a grey point group isomorphic to the white point group.

Rule 2: If the point group G_w contains a symmetry rotation θ about a direction $[xyz]$, then the rotation $\varphi=\theta/2$ (and its symmetry equivalent) about the direction $[xyz]$, *i.e.* $R=\{[xyz]/\varphi\}'$, gives rise to a composite point group $D=D_0+D_0R^{-1}$, where D_0 is the highest-order subgroup of G_w being invariant with R.

A special case of this rule is the following principle given by Pond & Bollmann (1979): 'colour-reversing rotation axes, u', can only be evenfold, and arise when two ordinary $u/2$-fold rotation axes coincide and θ is $2\pi/u$'.

Rule 3: For a mirror plane any rotation $\theta\neq 180°$ along a direction on the plane results in a colour-reversing mirror plane (or, in the case of improper rotation, in a twofold colour-reversing rotational axis), whereas for $\theta=180°$ an $mm'2'$ composite group is created.

Rule 4: In the case of two-, four- and sixfold ordinary rotational axes, rotation about a direction perpendicular to these axes results in a twofold colour-reversing rotational axis (or to a colour-reversing mirror plane in the case of improper rotations) except for some special rotation angles for which higher symmetry results due to the particular symmetry.

Rule 2 implies that in the particular case of a four- or sixfold ordinary axis special rotations (*i.e.* $\theta=2\pi/u$, $u=8$ or 12, respectively) create an eight- or 12-fold colour-reversing axis, respectively. Therefore, the superposition of ordinary point groups may result in noncrystallographic point groups and such groups are discussed in the following paper (Vlachavas, 1984). Here it is sufficient to notice that the symbolism of these groups follows the notation scheme of the senior crystallographic point groups. Also, we must mention that the 12-fold rotation and rotoinversion axes are designated for clarification by a line underneath their symbols.

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Two-Coloured Point and Rod Groups Containing an 8- or 12-fold Symmetry Axis

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Abstract

Lists of 8- and 12-fold two-coloured groups consistent with zero- and one-dimensional periodic objects are given. These groups are derived as extensions of the corresponding crystallographic two-coloured groups and are of particular interest because they are the only non-crystallographic groups obtained by the appropriate superposition of crystallographic point or rod groups.

1. Introduction

In the previous paper (Vlachavas, 1984) the symmetry of the composite obtained by the superposition of

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