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 $g_\alpha 1'g_i1'g_\alpha^{-1}=1'g_\alpha g_i g_\alpha^{-1}1'=g_j$ 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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two identical point groups with common origin was investigated. The two component groups, one designated white and the other black, were allowed to rotate relative to each other along any axis passing through their origin and the resulting symmetry was described in terms of antisymmetry (two-coloured symmetry) operations.

One of the main conclusions of the forementioned paper is the following rule: u-fold colour-reversing rotation axes arise when two ordinary $u/2$-fold rotation axes are coincident and the two component point groups are rotated relative to each other by $2\pi/u$ (see also Pond & Bollmann, 1979). This rule 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 8- or 12-fold colour-reversing axis, respectively. Thus, the superposition of identical point groups with common origin may yield non-crystallographic point groups of 8- and 12-fold colour-reversing symmetry and these groups are derived in §2.

Non-crystallographic rotation symmetry is also consistent with one-dimensional periodic objects provided that the 8- or 12-fold rotation axis is parallel to the periodicity direction (Pond & Bollmann, 1979; Vlachavas, 1980). Thus, in the last section of the paper we consider two-coloured rod groups containing non-crystallographic 8- or 12-fold rotational symmetry.

The symbols of the non-crystallographic symmetry elements considered here are built up according to the scheme explained by Vlachavas (1984). Thus, 8 and $\bar{8}$ denote 8-fold rotation and rotoinversion axes, respectively. In the case of 12-fold axes, however, the symbol 12 can be misinterpreted because of the possibility of confusing the 12-fold axis with the two-sided, one-coloured rosette group. The 12-fold axis is, therefore, designated by a line underneath the symbol, *i.e.* $\underline{12}$. Similarly, the 12-fold rotoinversion axis is represented by $\underline{\overline{12}}$.

2. Point groups containing 8- or 12-fold rotational symmetry

2.1. *One-coloured (ordinary) point groups*

Initially, the complete list of the ordinary point groups containing 8- or 12-fold symmetry operations is deduced. For this, combinations among the elements 8, $\bar{8}$, $\underline{12}$, $\underline{\overline{12}}$ and the crystallographic symmetry elements must be considered. The procedure for determining these combinations is similar to that yielding the 32 crystallographic point groups. Thus, applying the method of conventional crystallography (see *e.g.* Buerger, 1963), it is found that only combinations with two-fold rotational axes and mirror planes are permissible. Working on these lines the one-coloured point groups of 8- or 12-fold symmetry were derived and are given in the first column in Tables 1 and 2.

Table 1. *Antisymmetry point groups containing an ordinary or colour-reversing 8-fold axis*

Ordinary groups	Grey groups	Black–white groups
8	$81'$	$8'$
$\bar{8}$	$\bar{8}1'$	$\bar{8}'$
$8/m$	$8/m1'$	$8'/m$ $8/m'$ $8'/m'$
$8mm$	$8mm1'$	$8'mm'$ $8m'm'$
$\bar{8}m2$	$\bar{8}m21'$	$\bar{8}'m'2$ $\bar{8}'m2'$ $\bar{8}m'2'$
822	$8221'$	$8'22'$ $82'2'$
$8/mmm$	$8/mmm1'$	$8/m'm'm'$ $8'/mmm'$ $8/mm'm'$
		$8/m'mm$ $8'/m'm'm$

Table 2. *Antisymmetry point groups containing an ordinary or colour-reversing 12-fold axis*

Ordinary groups	Grey groups	Black–white groups
$\underline{12}$	$\underline{12}1'$	$\underline{12}'$
$\underline{\overline{12}}$	$\underline{\overline{12}}1'$	$\underline{\overline{12}}'$
$\underline{12}/m$	$\underline{12}/m1'$	$\underline{12}/m'$ $\underline{12}'/m$ $\underline{12}'/m'$
$\underline{12}mm$	$\underline{12}mm1'$	$\underline{12}m'm'$ $\underline{12}'mm'$
$\underline{\overline{12}}m2$	$\underline{\overline{12}}m21'$	$\underline{\overline{12}}m'2'$ $\underline{\overline{12}}'m2'$ $\underline{\overline{12}}'m'2$
$\underline{12}22$	$\underline{12}221'$	$\underline{12}2'2'$ $\underline{12}'22'$
$\underline{12}/mmm$	$\underline{12}/mmm1'$	$\underline{12}'/mmm'$ $\underline{12}'/m'mm'$ $\underline{12}/m'm'm'$
		$\underline{12}/m'mm$ $\underline{12}/mm'm'$

The new symbolism is built up on the following principles: each symbol gives from one to three symmetry elements which lie along special directions. These directions are: (i) the principal direction coincident with the non-crystallographic symmetry axis; (ii) the secondary direction perpendicular to the principal axis; and (iii) a direction which is also perpendicular to the principal axis and cuts the secondary axis at 22·5° (for the 8-fold groups) or 15° (for the 12-fold groups).

2.2. *Two-coloured point groups*

Having deduced the ordinary point groups we turn our attention to the complete enumeration of the corresponding grey and black–white point groups. This is carried out by employing the procedure proposed by Boyle (1969) for the construction of non-crystallographic two-coloured groups.

The basic principle of Boyle's procedure is the classification of the 32 ordinary point groups into families of 'halving subgroups' (*i.e.* subgroups which have half as many elements as the point group in question). The construction of non-crystallographic antisymmetry groups requires the extension of these 'family trees' downwards or the establishment of new ordinary groups without halving subgroups. In the particular case considered here, the 8- and 12-fold classes belong to the C_1 and C_3 families, respectively, and, therefore, the families are extended downwards. This is shown in Fig. 1, which is based on the corresponding diagrams given by Boyle (1969), but where the Hermann–Mauguin symbols are given instead of the Schönflies notation and the 8- and 12-fold ordinary groups are included. The horizontal rows contain groups of the same order and adjacent rows differ in order by a factor of two. The tie lines relate a group G to its halving subgroups H above and the groups of which it is halving subgroup below.

As has been shown by Boyle (1969), for any ordinary point group G there exists a grey group M given by $M = G + G1'$ (where $1'$ is the colour-identity operation) and a number of black–white point groups. The latter are defined by $M = H + (G - H)1'$, where H is a halving subgroup of G, and $(G - H)$ means the set of elements of G that do not belong to H. Thus, each tie line in Fig. 1 defines a black–white group. The lines connecting crystallographic point groups correspond to crystallographic black–white groups found by Tavger & Zaitsev (1956). The rest of the tie lines correspond to the non-crystallographic black–white point groups of 8- and 12-fold symmetry (Tables 1 and 2).

3. 8- and 12-fold rod groups

3.1. *Ordinary rod groups*

A figure without singular points and planes but with a singular axis is called a rod and the singular axis in it is called the axis of the rod. In addition to the translational axis, simple rotation, rotoinversion and screw axes of any order may coincide with the axis of the rod. The principle for the derivation of one-coloured symmetry groups of rods is based on the fact that rods cannot have inclined axes or symmetry planes, since these would give rise to several rod axes (by definition a rod can have only one singular or special axis). Hence, in order to derive all groups of rod symmetry only the types of symmetry applicable to figures with a singular point are used. Therefore, translational axes, screw axes or glide–reflection planes are located along the axis of the rod. Additional derivative symmetry elements (centres of symmetry, mirror planes and twofold axes perpendicular to the rod axis, and mirror–rotation axes coinciding with the axis of the rod) can arise. The translation symmetry for a rod is described by the one-dimensional net, *i.e.* the primitive one-dimensional lattice.

It is evident from the considerations above that the 8- or 12-fold axis must coincide with the rod axis. It is, thus, necessary to add the 8- or 12-fold point symmetry elements to the translation to obtain the possible rod groups. Hence, the screw axes corresponding to 8- or 12-fold rotations must initially be determined. These screw axes are characterized by the elementary angle $\varphi = 360°/8 = 45°$ or $360°/12 = 30°$, respectively, and also by the screw translation $\tau = (j/n)t$, where t is the elementary translation along the axis of the rod, n is equal to 8 or 12 and j is the pitch component of the screw axis. The screw axes isogonal with the 8- and 12-fold rotation axes are given below, grouped in pairs of enantiomorphic

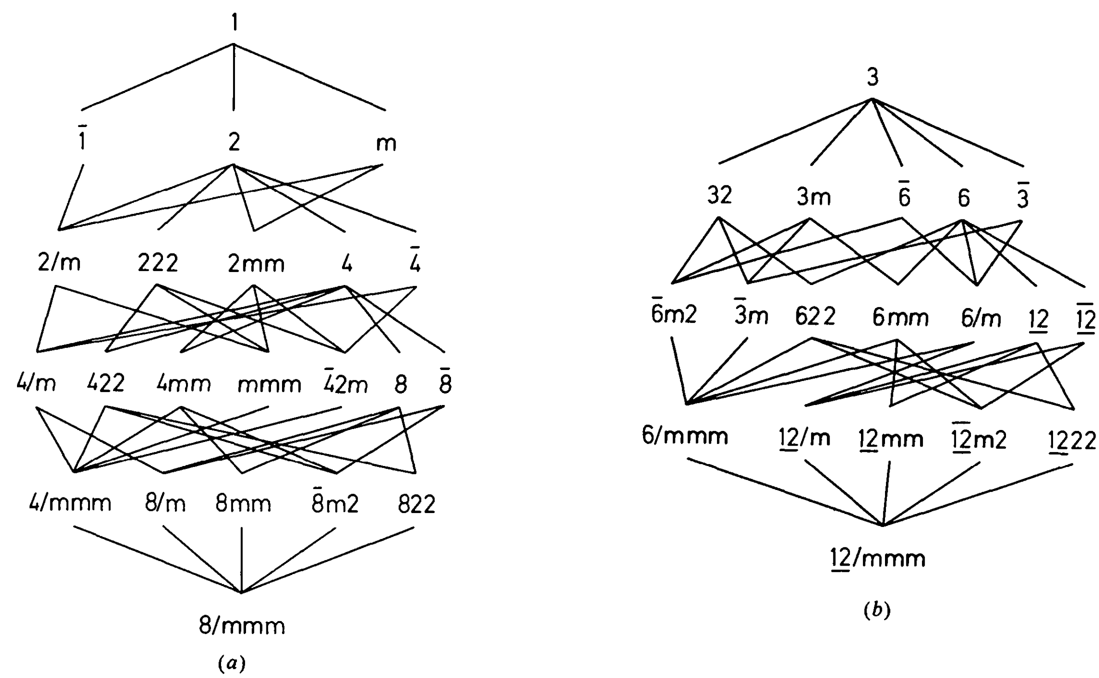

Fig. 1. The 'family trees' of (one-coloured) point symmetries used for the construction of two-coloured non-crystallographic point groups of 8- and 12-fold symmetry: (*a*) the C_1 family, (*b*) the C_3 family.

Table 3. *Antisymmetry rod groups containing an 8-fold symmetry axis*

Rod-group symbol

No.	One-coloured groups	Two-coloured groups: Grey groups	Black–white groups: Without antitranslation	Black–white groups: With antitranslation
1	$\not{p}8$	$\not{p}81'$	$\not{p}8'$	$\not{p}'8$
2	$\not{p}8_1$	$\not{p}8_11'$	$\not{p}8'_1$	$\not{p}'8_1$
3	$\not{p}8_2$	$\not{p}8_21'$	$\not{p}8'_2$	$\not{p}'8_2$
4	$\not{p}8_3$	$\not{p}8_31'$	$\not{p}8'_3$	$\not{p}'8_3$
5	$\not{p}8_4$	$\not{p}8_41'$	$\not{p}8'_4$	$\not{p}'8_4$
6	$\not{p}8_5$	$\not{p}8_51'$	$\not{p}8'_5$	$\not{p}'8_5$
7	$\not{p}8_6$	$\not{p}8_61'$	$\not{p}8'_6$	$\not{p}'8_6$
8	$\not{p}8_7$	$\not{p}8_71'$	$\not{p}8'_7$	$\not{p}'8_7$
9	$\not{p}\bar{8}$	$\not{p}\bar{8}1'$	$\not{p}\bar{8}'$	$\not{p}'\bar{8}$
10	$\not{p}8/m$	$\not{p}8/m1'$	$\not{p}8'/m$, $\not{p}8/m'$, $\not{p}8'/m'$	$\not{p}'8/m$
11	$\not{p}8_4/m$	$\not{p}8_4/m1'$	$\not{p}8'_4/m$, $\not{p}8_4/m'$, $\not{p}8'_4/m'$	$\not{p}'8_4/m$
12	$\not{p}8mm$	$\not{p}8mm1'$	$\not{p}8'mm'$, $\not{p}8m'm'$	$\not{p}'8mm$
13	$\not{p}8cc$	$\not{p}8cc1'$	$\not{p}8'cc'$, $\not{p}8c'c'$	$\not{p}'8cc$
14	$\not{p}8_4mc$	$\not{p}8_4mc1'$	$\not{p}8_4m'c'$, $\not{p}8'_4mc'$, $\not{p}8'_4m'c$	$\not{p}'8_4mc$
15	$\not{p}822$	$\not{p}8221'$	$\not{p}8'22'$, $\not{p}82'2'$	$\not{p}'822$
16	$\not{p}8_122$	$\not{p}8_1221'$	$\not{p}8'_122'$, $\not{p}8_12'2'$	$\not{p}'8_122$
17	$\not{p}8_222$	$\not{p}8_2221'$	$\not{p}8'_222'$, $\not{p}8_22'2'$	$\not{p}'8_222$
18	$\not{p}8_322$	$\not{p}8_3221'$	$\not{p}8'_322'$, $\not{p}8_32'2'$	$\not{p}'8_322$
19	$\not{p}8_422$	$\not{p}8_4221'$	$\not{p}8'_422'$, $\not{p}8_42'2'$	$\not{p}'8_422$
20	$\not{p}8_522$	$\not{p}8_5221'$	$\not{p}8'_522'$, $\not{p}8_52'2'$	$\not{p}'8_522$
21	$\not{p}8_622$	$\not{p}8_6221'$	$\not{p}8'_622'$, $\not{p}8_62'2'$	$\not{p}'8_622$
22	$\not{p}8_722$	$\not{p}8_7221'$	$\not{p}8'_722'$, $\not{p}8_72'2'$	$\not{p}'8_722$
23	$\not{p}\bar{8}2m$	$\not{p}\bar{8}2m1'$	$\not{p}\bar{8}'2m'$, $\not{p}\bar{8}'2'm$, $\not{p}\bar{8}2'm'$	$\not{p}'\bar{8}2m$
24	$\not{p}\bar{8}2c$	$\not{p}\bar{8}2c1'$	$\not{p}\bar{8}'2c'$, $\not{p}\bar{8}'2'c$, $\not{p}\bar{8}2'c'$	$\not{p}'\bar{8}2c$
25	$\not{p}8/mmm$	$\not{p}8/mmm1'$	$\not{p}8/m'm'm'$, $\not{p}8'/mmm'$, $\not{p}8/mm'm'$, $\not{p}8/m'mm$, $\not{p}8'/m'mm'$	$\not{p}'8/mmm$
26	$\not{p}8_4/mcm$	$\not{p}8_4/mcm1'$	$\not{p}8_4/m'c'm'$, $\not{p}8'_4/mcm'$, $\not{p}8'_4/mc'm$, $\not{p}8_4/mc'm'$, $\not{p}8_4/m'cm$, $\not{p}8'_4/m'cm'$, $\not{p}8'_4/m'c'm$	$\not{p}'8_4/mcm$
27	$\not{p}8/mcc$	$\not{p}8/mcc1'$	$\not{p}8/m'c'c'$, $\not{p}8'/mcc'$, $\not{p}8/mc'c'$, $\not{p}8/m'cc$, $\not{p}8'/m'cc'$	$\not{p}'8/mcc$

Table 4. *Antisymmetry rod groups containing a 12-fold symmetry axis*

Rod-group symbol

No.	One-coloured groups	Two-coloured groups: Grey groups	Black–white groups: Without antitranslation	Black–white groups: With antitranslation
1	$\not{p}\underline{12}$	$\not{p}\underline{12}1'$	$\not{p}\underline{12}'$	$\not{p}'\underline{12}$
2	$\not{p}\underline{12}_1$	$\not{p}\underline{12}_11'$	$\not{p}\underline{12}'_1$	$\not{p}'\underline{12}_1$
3	$\not{p}\underline{12}_2$	$\not{p}\underline{12}_21'$	$\not{p}\underline{12}'_2$	$\not{p}'\underline{12}_2$
4	$\not{p}\underline{12}_3$	$\not{p}\underline{12}_31'$	$\not{p}\underline{12}'_3$	$\not{p}'\underline{12}_3$
5	$\not{p}\underline{12}_4$	$\not{p}\underline{12}_41'$	$\not{p}\underline{12}'_4$	$\not{p}'\underline{12}_4$
6	$\not{p}\underline{12}_5$	$\not{p}\underline{12}_51'$	$\not{p}\underline{12}'_5$	$\not{p}'\underline{12}_5$
7	$\not{p}\underline{12}_6$	$\not{p}\underline{12}_61'$	$\not{p}\underline{12}'_6$	$\not{p}'\underline{12}_6$
8	$\not{p}\underline{12}_7$	$\not{p}\underline{12}_71'$	$\not{p}\underline{12}'_7$	$\not{p}'\underline{12}_7$
9	$\not{p}\underline{12}_8$	$\not{p}\underline{12}_81'$	$\not{p}\underline{12}'_8$	$\not{p}'\underline{12}_8$
10	$\not{p}\underline{12}_9$	$\not{p}\underline{12}_91'$	$\not{p}\underline{12}'_9$	$\not{p}'\underline{12}_9$
11	$\not{p}\underline{12}_{10}$	$\not{p}\underline{12}_{10}1'$	$\not{p}\underline{12}'_{10}$	$\not{p}'\underline{12}_{10}$
12	$\not{p}\underline{12}_{11}$	$\not{p}\underline{12}_{11}1'$	$\not{p}\underline{12}'_{11}$	$\not{p}'\underline{12}_{11}$
13	$\not{p}\overline{\underline{12}}$	$\not{p}\overline{\underline{12}}1'$	$\not{p}\overline{\underline{12}}'$	$\not{p}'\overline{\underline{12}}$
14	$\not{p}\underline{12}/m$	$\not{p}\underline{12}/m1'$	$\not{p}\underline{12}'/m$, $\not{p}\underline{12}/m'$, $\not{p}\underline{12}'/m'$	$\not{p}'\underline{12}/m$
15	$\not{p}\underline{12}_6/m$	$\not{p}\underline{12}_6/m1'$	$\not{p}\underline{12}'_6/m$, $\not{p}\underline{12}_6/m'$, $\not{p}\underline{12}'_6/m'$	$\not{p}'\underline{12}_6/m$
16	$\not{p}\underline{12}mm$	$\not{p}\underline{12}mm1'$	$\not{p}\underline{12}'mm'$, $\not{p}\underline{12}m'm'$	$\not{p}'\underline{12}mm$
17	$\not{p}\underline{12}cc$	$\not{p}\underline{12}cc1'$	$\not{p}\underline{12}'cc'$, $\not{p}\underline{12}c'c'$	$\not{p}'\underline{12}cc$
18	$\not{p}\underline{12}_6mc$	$\not{p}\underline{12}_6mc1'$	$\not{p}\underline{12}_6m'c'$, $\not{p}\underline{12}'_6mc'$, $\not{p}\underline{12}'_6m'c$	$\not{p}'\underline{12}_6mc$
19	$\not{p}\underline{12}22$	$\not{p}\underline{12}221'$	$\not{p}\underline{12}'22'$, $\not{p}\underline{12}2'2'$	$\not{p}'\underline{12}22$
20	$\not{p}\underline{12}_122$	$\not{p}\underline{12}_1221'$	$\not{p}\underline{12}'_122'$, $\not{p}\underline{12}_12'2'$	$\not{p}'\underline{12}_122$
21	$\not{p}\underline{12}_222$	$\not{p}\underline{12}_2221'$	$\not{p}\underline{12}'_222'$, $\not{p}\underline{12}_22'2'$	$\not{p}'\underline{12}_222$
22	$\not{p}\underline{12}_322$	$\not{p}\underline{12}_3221'$	$\not{p}\underline{12}'_322'$, $\not{p}\underline{12}_32'2'$	$\not{p}'\underline{12}_322$
23	$\not{p}\underline{12}_422$	$\not{p}\underline{12}_4221'$	$\not{p}\underline{12}'_422'$, $\not{p}\underline{12}_42'2'$	$\not{p}'\underline{12}_422$
24	$\not{p}\underline{12}_522$	$\not{p}\underline{12}_5221'$	$\not{p}\underline{12}'_522'$, $\not{p}\underline{12}_52'2'$	$\not{p}'\underline{12}_522$
25	$\not{p}\underline{12}_622$	$\not{p}\underline{12}_6221'$	$\not{p}\underline{12}'_622'$, $\not{p}\underline{12}_62'2'$	$\not{p}'\underline{12}_622$
26	$\not{p}\underline{12}_722$	$\not{p}\underline{12}_7221'$	$\not{p}\underline{12}'_722'$, $\not{p}\underline{12}_72'2'$	$\not{p}'\underline{12}_722$
27	$\not{p}\underline{12}_822$	$\not{p}\underline{12}_8221'$	$\not{p}\underline{12}'_822'$, $\not{p}\underline{12}_82'2'$	$\not{p}'\underline{12}_822$
28	$\not{p}\underline{12}_922$	$\not{p}\underline{12}_9221'$	$\not{p}\underline{12}'_922'$, $\not{p}\underline{12}_92'2'$	$\not{p}'\underline{12}_922$
29	$\not{p}\underline{12}_{10}22$	$\not{p}\underline{12}_{10}221'$	$\not{p}\underline{12}'_{10}22'$, $\not{p}\underline{12}_{10}2'2'$	$\not{p}'\underline{12}_{10}22$
30	$\not{p}\underline{12}_{11}22$	$\not{p}\underline{12}_{11}221'$	$\not{p}\underline{12}'_{11}22'$, $\not{p}\underline{12}_{11}2'2'$	$\not{p}'\underline{12}_{11}22$
31	$\not{p}\overline{\underline{12}}2m$	$\not{p}\overline{\underline{12}}2m1'$	$\not{p}\overline{\underline{12}}'2m'$, $\not{p}\overline{\underline{12}}'2'm$, $\not{p}\underline{12}2'm'$	$\not{p}'\overline{\underline{12}}2m$
32	$\not{p}\overline{\underline{12}}2c$	$\not{p}\overline{\underline{12}}2c1'$	$\not{p}\overline{\underline{12}}'2c'$, $\not{p}\overline{\underline{12}}'2'c$, $\not{p}\overline{\underline{12}}2'c'$	$\not{p}'\overline{\underline{12}}2c$
33	$\not{p}\underline{12}/mmm$	$\not{p}\underline{12}/mmm1'$	$\not{p}\underline{12}/m'm'm'$, $\not{p}\underline{12}'/mmm'$, $\not{p}\underline{12}/mm'm'$, $\not{p}\underline{12}/m'mm$, $\not{p}\underline{12}'/m'mm'$	$\not{p}'\underline{12}/mmm$
34	$\not{p}\underline{12}_6/mcm$	$\not{p}\underline{12}_6/mcm1'$	$\not{p}\underline{12}_6/m'c'm'$, $\not{p}\underline{12}'_6/mcm'$, $\not{p}\underline{12}'_6/mc'm$, $\not{p}\underline{12}_6/mc'm'$, $\not{p}\underline{12}_6/m'cm$, $\not{p}\underline{12}'_6/m'cm'$, $\not{p}\underline{12}'_6/m'c'm$	$\not{p}'\underline{12}_6/mcm$
35	$\not{p}\underline{12}/mcc$	$\not{p}\underline{12}/mcc1'$	$\not{p}\underline{12}/m'c'c'$, $\not{p}\underline{12}'/mcc'$, $\not{p}\underline{12}/mc'c'$, $\not{p}\underline{12}/m'cc$, $\not{p}\underline{12}'/m'cc'$	$\not{p}'\underline{12}/mcc$

symmetry (except the neutral axes):

8-fold screw axes: $(8_1, 8_7)$, $(8_2, 8_6)$, $(8_3, 8_5)$, 8_4

12-fold screw axes: $(\underline{12}_1, \underline{12}_{11})$, $(\underline{12}_2, \underline{12}_{10})$, $(\underline{12}_3, \underline{12}_9)$, $(\underline{12}_4, \underline{12}_8)$, $(\underline{12}_5, \underline{12}_7)$, $\underline{12}_6$.

When the operations of the 8- and 12-fold point symmetry and translation (including screw axes and glide planes) are taken into account, the one-coloured rod groups can be derived; they are listed in Tables 3 and 4 under the heading 'one-coloured groups'. In these tables the symbol of the one-dimensional lattice is given first; the letter or number in the second, third and fourth positions of the symbol indicate that a particular symmetry element coincides with the coordinate axes **a**, **b** and the bisector of the angle between the axes **b** and **c**. If no symmetry axis or normal to symmetry plane coincides with the coordinate axis the corresponding position is left vacant (short symbol). The coordinate axis **a** is directed along the rod axis, and the axes **b** and **c** are orthogonal to the axis **a** and make a 22·5 or 15° angle with each other, depending on the class of the rod symmetry (8- or 12-fold, respectively).

3.2. *Two-coloured rod groups*

The two-coloured rod groups containing an 8- or 12-fold axis are presented in Tables 3 and 4, respectively. The first column in these tables gives the symbols of the one-coloured rod groups derived above. The second column gives the symbols of the grey (neutral) groups obtained by additing the anti-identity operation 1′ to the generators of the one-coloured groups (Belov & Tarkhova, 1956). All the grey groups can accordingly be considered as extensions of the classical groups by means of the group 1′. Thus, if we denote by C and D the classical and two-coloured rod groups we have that $D = C \otimes 1'$ for the grey groups.

The third column of the tables gives the symbols of the black–white groups D isomorphic with the one-coloured groups C listed in the first columns of the tables. These D groups, which do not contain any antitranslation, may be regarded as extensions of the classical subgroups $C^* \subset C$ of index 2 by means of the antisymmetry point groups G' or antisymmetry groups by modulus $G^{T'}$, *i.e.* as direct, semidirect and quasi-direct products (see *e.g.* Shubnikov & Koptsik, 1974):

$$D = C^* \otimes G', \qquad D = C^* \circledS G' \quad \text{or} \quad D = C^* \odot G^{T'}.$$

Thus, for example, $\not{p}8' = \not{p}4 \otimes 2'$, $\not{p}\underline{12}m'm' = \not{p}\underline{12} \circledS m'$ and $\not{p}8'/m = \not{p}4/m \odot 8'(\mathrm{mod}\ 2)$.

Finally, the two-coloured rod groups in the last column of Tables 3 and 4 contain antitranslations τ'. These groups are obtained from the one-coloured rod groups by additing to the generators of the translation subgroup $T \subset C$ an antitranslation generator τ'. Groups of this type may thus be considered as extensions of the classical groups $C^* = TG$ by means of the group by modulus $\tau'(\mathrm{mod}\ 2\tau) = \{1, \tau'\}$.

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Experimental Study of X-ray Diffraction under Specular Reflection Conditions

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Abstract

Results of the experimental study of X-ray diffraction under specular reflection conditions are presented. The experimental arrangement which permits the measurement of the intensity of a specularly reflected diffracted wave with respect to its exit angle to the crystal surface is described. Experimental confirmation of the theory [Afanas'ev & Melkonyan (1983). *Acta Cryst.* **A39**, 207–210] has been obtained for silicon crystals. The angular distributions of the specularly reflected and diffuse intensities have also been studied. The experiments showed the diffuse scattering to be primarily scattering at the back edge of the sample.

The diffraction under specular reflection conditions occurs when an X-ray beam is directed into a crystal at a small glancing angle, φ, of incidence comparable with the critical angle of specular reflection and, simultaneously, if the conditions of Laue case diffraction for the planes normal to the surface are met.

As was shown earlier (Marra, Eisenberger & Cho, 1979; Afanas'ev & Melkonyan, 1983), two specularly

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