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Layer and Rod Classes of Reducible Space Groups. II. *Z*-Reducible Cases

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Abstract

Reducible plane groups of rectangular systems with *c* lattices are classified into frieze classes and reducible space groups with centered lattices are classified into layer and rod classes with respect to those *Q* reductions that lead to *Z* reduction but not to *Z* decomposition. Tables are given for plane groups, presenting their homomorphic projections onto frieze groups, and for space groups, presenting their homomorphic projections onto layer and rod groups. These projections define the classes to which the plane and space groups belong. In both cases, the characteristic shift vectors are listed that change the plane or space group without changing the homomorphic projections onto frieze, layer and rod groups.

1. Introduction

In the established terminology of integral representations of finite groups [Curtis & Reiner (1966); in a crystallographic context: Brown, Bülow, Neubüser, Wondratschek & Zassenhaus (1978)], *Z* decomposition is a special case of *Z* reduction. In paper I of this series (Kopský, 1993), the frieze classes of reducible plane groups and layer and rod classes of reducible space groups with respect to those *Z* reductions that are *Z* decompositions were tabulated. To complete the distribution of reducible space groups into layer and rod classes (plane groups into pairs of frieze classes), we consider now the cases of those *Z* reductions that are not *Z* decompositions. For simplicity, we shall use the term *Z* reduction to mean only those that are not *Z* decompositions if we do not state otherwise.

The classification of reducible space groups with respect to *Z* reductions has a few specific features that distinguish it from the classification with respect to *Z* decompositions. This is one of the reasons for considering them separately.

Classification into layer and rod classes (or into pairs of frieze classes) is equivalent to factorization by partial translation subgroups or to determination of corresponding homomorphic projections. The latter are more suitable for *Z* reductions. To avoid misunderstanding, let us observe that the projections we talk about are not identical with the special projections listed in *International Tables for Crystallography* (1987).

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2. Z reductions and centered lattices

Z decomposition of a translation group is a decomposition into a direct sum of translation subgroups, while Z reduction refers to a subdirect sum, where a direct sum is again a special case of the subdirect sum. Accordingly, we use the term subdirect sum below only in cases that do not imply a direct sum, if not stated otherwise. There is, furthermore, a close relationship between Z reductions or subdirect sums and centered lattices that is worthy of dimension-independent study. We will now see how reductions are related to lattice types up to three dimensions.

Crystallographers conventionally tend to consider the difference between primitive and centered lattices. Let us consider the p and c types of rectangular lattices in the plane as described in the book by Brown, Bülow, Neubüser, Wondratschek & Zassenhaus (1978). Clearly, if we take vectors $(\mathbf{a}+\mathbf{b})/2$, $(\mathbf{a}-\mathbf{b})/2$ as a new conventional basis, then the primitive and centered cases exchange their roles. We have, however, a strong reason to prefer the choice of vectors $\mathbf{a}$ and $\mathbf{b}$ as the conventional basis: the translation subgroups $T(\mathbf{a})$, $T(\mathbf{b})$ that they generate are invariant under the action of rectangular point groups, while the groups $T[(\mathbf{a}+\mathbf{b})/2]$, $T[(\mathbf{a}-\mathbf{b})/2]$ are not. However, this reasoning cannot be applied to cubic lattices of the three types P, F and I, where all corresponding translation groups are irreducible under the action of cubic groups.

In any case, the conventions are such that all lattices of Bravais p type in the plane or of P type in three dimensions imply Z decomposition under the action of a reducible point group. There is only one centered type in the plane, the c type, which leads to Z reduction. In three dimensions we have three centered types - base centered (A, B or C), volume centered (I) and face centered (F). The symbols A, B, C express the same centering with respect to various settings.

For C centering, the centering vector lies in the plane $V(\mathbf{a}, \mathbf{b})$ and the translation group is expressible as the direct sum of the translation group in the plane (centered plane lattice) and the translation group generated by vector $\mathbf{c}$. The cases of C centering appear only in inclined reductions of monoclinic groups and in reductions of orthorhombic groups; factorization by $T(\mathbf{c})$ leads to layer groups with rectangular c-centered lattices. All these cases are recorded in tables in paper I (Kopský, 1993).

The rhombohedral lattice (R) is a special case. It is primitive in the rhombohedral basis. The corresponding translation group is Z reducible but the reduction is expressed better in the hexagonal basis, in which the lattice can be considered as centered hexagonal.

Z decomposition and Z reduction as well as direct or subdirect sums are established mathematical concepts, the meanings of which are clear in any dimension. The concept of centered lattices is a conventional concept, introduced on the basis of experience with three-dimensional crystallography and its meaning in arbitrary dimensions is thus far not entirely clear.

3. Specific features of factorization with respect to Z reductions

For Z reductions, the translation subgroup T_G of the space group invariably splits into a subdirect sum

$$T_G = T_{G1} \oplus T_{G2}[\mathbf{0} \cup \mathbf{d}_2 \cup \ldots \cup \mathbf{d}_p]$$

and the projections

$$T^0_{G1} = T_{G1}[\mathbf{0} \cup \mathbf{d}_{21} \cup \ldots \cup \mathbf{d}_{p1}],$$

$$T^0_{G2} = T_{G2}[\mathbf{0} \cup \mathbf{d}_{22} \cup \ldots \cup \mathbf{d}_{p2}]$$

appear as translation subgroups of the factor groups $\mathbb{L} = \boldsymbol{\sigma}_1(\mathbb{G})$, $\mathbb{R} = \boldsymbol{\sigma}_2(\mathbb{G})$, respectively. The Z decompositions occur as special cases of Z reductions, when $T_G = T_{G1} \oplus T_{G2}$, $T_{G1} = T^0_{G1}$, $T_{G2} = T^0_{G2}$. The group

$$T_{G0} = T_{G1} \oplus T_{G2}$$

is the translation group that defines the conventional unit cell for Z decompositions and Z reductions. Thus it corresponds to the group $T(\mathbf{a}, \mathbf{b})$ in planar cases and $T(\mathbf{a}, \mathbf{b}, \mathbf{c})$ in three-dimensional cases, where $\mathbf{a}, \mathbf{b}, \mathbf{c}$ are the vectors of the conventional basis. For Z decomposition, the group T_{G0} coincides with the group T_G; for Z reduction, T_{G0} is a subgroup of T_G and the centering vectors $\mathbf{d}_i$, $i = 1, 2, \ldots, p$, are representatives of coset resolution of T_G *versus* T_{G0}. There are three main practically immediate and interrelated consequences that distinguish Z-reducible cases from Z-decomposable ones.

1. The symmorphic representative of a subperiodic class is never associated with Z reduction. Clearly, the symmorphic representative, as a semidirect product, must contain the (copy of the) layer or rod group of the class it represents as its subgroup. This is impossible here because the space group does not even contain the translation subgroups T^0_{G1}, $T^0_{G_2}$ of groups $\mathbb{L}$ and $\mathbb{R}$. From the viewpoint of group-extension theory (Ascher & Janner, 1965, 1968/1969), the projections of centering vectors $\mathbf{d}_{j1}$, $\mathbf{d}_{j2}$ may be interpreted as mutual nonprimitive translations.

2. Homomorphic projections of standard space groups with respect to Z reductions never result in standard subperiodic groups. Either the setting or, at least, the lengths of standard vectors of the conventional basis are different. Indeed, if vectors $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ define the standard conventional cell of the space groups of some system then vectors $\mathbf{a}$ and $\mathbf{b}$ define the standard conventional cell of the corresponding layer groups, vector $\mathbf{c}$ the standard conventional cell of the corresponding rod groups. This corresponds to the Z decomposition $T_G = T(\mathbf{a}, \mathbf{b}, \mathbf{c}) = T(\mathbf{a}, \mathbf{b}) \oplus$

$T(\mathbf{c}) = T_{G1} \oplus T_{G2}$. While, for Z decompositions, $T_{G1} = T^0_{G1} = \sigma_1(T_G)$ and $T_{G2} = T^0_{G2} = \sigma_2(T_G)$, for Z reductions, $T_{G1} \subset T^0_{G1} = \sigma_1(T_G)$ and $T_{G2} \subset T^0_{G2} = \sigma_2(T_G)$. The conventional cells of projected groups are therefore smaller than in the case of Z decompositions.

3. The intersection theorem does not hold for Z reductions. The pair of a layer and a rod group of the same geometric class, with translation subgroups T^0_{G1}, T^0_{G2}, respectively, uniquely determines a space group of this geometric class with translation subgroup $T^0_G = T^0_{G1} \oplus T^0_{G2}$ since the sum of nonprimitive translations that satisfy Frobenius congruences mod T^0_{G1} and T^0_{G2}, respectively, satisfies Frobenius congruences mod T^0_G. In view of additional conditions [equation (8*a*) of (Kopský (1989*a*)], it may or may not satisfy the congruences mod T_G and hence it may happen that a pair of subperiodic groups does not determine any space group with the translation subgroups T_G. However, theorem 3 of Kopský (1989*b*) shows that such a pair may define several space groups of the same type, differing by so-called 'characteristic shift vectors'.

4. Translation normalizers and characteristic shift vectors

The shift of a space group $\mathbb{G} = \{G, T_G, P, \mathbf{u}_G(g)\}$ in space by a vector $\boldsymbol{\tau}$ leads to a group $\mathbb{G}(\boldsymbol{\tau}) = \{G, T_G, P+\boldsymbol{\tau}, \mathbf{u}_G(g)\}$. The shift can also be expressed by the change of the system of nonprimitive translations with respect to the origin P by the so-called 'shift function' $\boldsymbol{\varphi}(g, \boldsymbol{\tau}) = \boldsymbol{\tau} - g\boldsymbol{\tau}$, so that the shifted group is expressed as $\mathbb{G}(\boldsymbol{\tau}) = \{G, T_G, P, \mathbf{u}_G(g) + \boldsymbol{\varphi}(g, \boldsymbol{\tau})\}$. If the shift $\boldsymbol{\tau}$ satisfies the condition $\boldsymbol{\varphi}(g, \boldsymbol{\tau}) \in T_G$ for all $g \in G$, which can be expressed in the form of congruences $\boldsymbol{\varphi}(g, \boldsymbol{\tau}) = \mathbf{0} \bmod T_G$, then $\mathbb{G}(\boldsymbol{\tau}) = \mathbb{G}$. All vectors $\boldsymbol{\tau}$ that satisfy these conditions and hence do not change the group $\mathbb{G}$ form a so-called 'translation normalizer' $T_N(\mathbb{G}) = T_N(G, T_G)$ of the group $\mathbb{G}$. The symbol $T_N(G, T_G)$ refers to the fact that all groups of the arithmetic class (G, T_G) have the same translation normalizer. The latter occur as translation subgroups of affine and Euclidean normalizers [Wondratschek's contribution to *International Tables for Crystallography* (1987)]. They can be easily deduced from space-group diagrams (Hirshfeld, 1968) and they are themselves of both interest and importance in more general contexts (Kopský, 1992).

If the projections of space group $\mathbb{G}$ are the layer group $\mathbb{L} = \boldsymbol{\sigma}_1(\mathbb{G})$ and the rod group $\mathbb{R} = \boldsymbol{\sigma}_2(\mathbb{G})$, then the projections of the group $\mathbb{G}(\boldsymbol{\tau})$ are the layer group $\mathbb{L}(\boldsymbol{\tau}_1)$ and the rod group $\mathbb{R}(\boldsymbol{\tau}_2)$, where $\boldsymbol{\tau}_1 = \sigma_1(\boldsymbol{\tau})$, $\boldsymbol{\tau}_2 = \sigma_2(\boldsymbol{\tau})$ are projections of shift vector $\boldsymbol{\tau}$. The layer group $\mathbb{L}(\boldsymbol{\tau}_1)$ coincides with $\mathbb{L}$ only if $\boldsymbol{\tau}_1$ is a vector of the translation normalizer $T_N(\mathbb{L}) = T_N(G, T^0_{G1})$ and the rod group $\mathbb{R}(\boldsymbol{\tau}_2)$ coincides with $\mathbb{R}$ only if $\boldsymbol{\tau}_2$ is a vector of the translation normalizer $T_N(\mathbb{R}) = T_N(G, T^0_{G2})$.

For Z decompositions, $T_N(\mathbb{G}) = T_N(\mathbb{L}) \oplus T_N(\mathbb{R})$ and if a shift $\boldsymbol{\tau}$ leads to a group $\mathbb{G}(\boldsymbol{\tau})$ distinct from $\mathbb{G}$ then its projections $\boldsymbol{\tau}_1$, $\boldsymbol{\tau}_2$ lead to layer and rod groups $\mathbb{L}(\boldsymbol{\tau}_1)$ and $\mathbb{R}(\boldsymbol{\tau}_2)$ distinct from $\mathbb{L}$ and $\mathbb{R}$, respectively. This follows from $T_{G1} = T^0_{G1}$ and $T_{G2} = T^0_{G2}$. For Z reductions, we still have $T_N(\mathbb{L}) = T_N(G, T^0_{G1})$, $T_N(\mathbb{R}) = T_N(G, T^0_{G2})$, but now $T_{G1} \subset T^0_{G1}$ and $T_{G2} \subset T^0_{G2}$ and often $T_N(\mathbb{G}) \subset T_N(\mathbb{L}) \oplus T_N(\mathbb{R})$. Let us now consider the coset resolution:

$$T_N(\mathbb{L}) \oplus T_N(\mathbb{R}) = T_N(\mathbb{G})[\mathbf{0} \cup \mathbf{q}_2 \cup \ldots \cup \mathbf{q}_S],$$

where $\mathbf{q}_i$ are the characteristic shift vectors. These have the property that $\mathbb{L}(\mathbf{q}_i) = \mathbb{L}$ and $\mathbb{R}(\mathbf{q}_i) = \mathbb{R}$ but $\mathbb{G}(\mathbf{q}_i) \neq \mathbb{G}$. Hence the shift of a space group $\mathbb{G}$ by $\mathbf{q}_i$ leads to a group $\mathbb{G}(\mathbf{q}_i)$, of the same type and parameters as $\mathbb{G}$, but of a different location in space, while homomorphic projections of both groups $\mathbb{G}$ and $\mathbb{G}(\mathbf{q}_i)$ are identical.

5. Factorization procedure for Z reductions

As in the case of Z decompositions, we can perform the factorization procedure either algebraically or with the use of relevant space-group diagrams. In the first step of algebraic factorization, we determine the components of the system of nonprimitive translations of the space group $\mathbb{G}$ in subspaces $V(\mathbf{a}, \mathbf{b})$ and $V(\mathbf{c})$ in terms of the conventional basis vectors of groups T^0_{G1} and T^0_{G2}. By comparing these with standards, we get the subperiodic factor groups.

Factorization with use of space-group diagrams is direct, more appealing for crystallographers and it has some new features in comparison with Z-decomposable cases. The direct sum $T_{G0} = T_{G1} \oplus T_{G2} = T(\mathbf{a}, \mathbf{b}, \mathbf{c})$ defines the conventional unit cell (in a trigonal system this is the hexagonal cell) and the graphical symbols refer to this cell. For example, the dotted line again means a glide plane with glide translation $\mathbf{c}/2$. The centering vectors $\mathbf{d}_i$ are elements of the translation group T_G and hence they combine with every operation $\{g|\mathbf{t}\}$, $\mathbf{t} \in T_{G0} = T(\mathbf{a}, \mathbf{b}, \mathbf{c})$. The addition of the centering vector brings a shift of the symmetry element in space and adds a screw or glide translation to it, depending on the type and orientation of the operation g. Symmetry elements then appear in couples (A, B, C and I centerings), triplets (rhombohedral lattice R) or even quartets (F centering) and the simple rules for converting the diagram of a space group into those of its factor layer and rod groups do not always hold. We can clearly see this from diagrams where, in some cases, new graphical symbols must be introduced that are not present in diagrams of groups with P-type lattices. The diamond plane is a spectacular example. Connected with this is some uncertainty in the Hermann–Mauguin symbols, which are not uniquely justified, which was the case for the P lattices, and for which several equally logical symbols can be introduced. We shall give more

Table 1. *Homomorphisms of reducible plane groups onto frieze groups with respect to Z reductions*

	$\sigma_{\mathbf{a}}$	$\sigma_{\mathbf{b}}$	$\mathbf{q}$
$c1m1$	$\not{p}_{\mathbf{a}/2}1m1$	$\not{p}_{\mathbf{b}/2}11m$	$0, \mathbf{a}/4$
$c11m$	$\not{p}_{\mathbf{a}/2}11m$	$\not{p}_{\mathbf{b}/2}1m1$	$0, \mathbf{b}/4$
$c2mm$	$\not{p}_{\mathbf{a}/2}2mm$	$\not{p}_{\mathbf{b}/2}2mm$	$0, \mathbf{a}/4, \mathbf{b}/4, (\mathbf{a}+\mathbf{b})/4$

attention to these new features through comments on individual systems in the next section.

6. Homomorphic projections of reducible plane and space groups with respect to Z reductions

In tables of homomorphic projections we use the standards of reducible plane and of reducible space groups so that the resulting projections are not standard. We shall therefore arrange the tables in a different way. In the first column of each table we list the Schönflies symbols for the point classes; in the next column these are followed by the Schönflies symbols of the corresponding reducible space groups for which Z reduction of the translation subgroup occurs. For monoclinic and orthorhombic groups we list further the Hermann–Mauguin symbols of these groups in all settings (in monoclinic cases we should consider the type of the setting) that imply Z reduction. Homomorphic projections are listed in the next two columns, where the indices of the symbols $\boldsymbol{\sigma}$ denote the plane or line onto which we project. The last column contains all characteristic shift vectors. We also list all information conventionally with respect to the R reduction $V(\mathbf{a}, \mathbf{b}) \oplus V(\mathbf{c})$, so that the layer groups are always related to the space $E(\mathbf{a}, \mathbf{b}) \times V(\mathbf{c})$.

Plane groups of a rectangular system. The unique centered lattice type in the plane is the c-rectangular type. The homomorphisms $\boldsymbol{\sigma}_{\mathbf{a}}$, $\boldsymbol{\sigma}_{\mathbf{b}}$ of the two group types (one in two settings) onto frieze groups and the characteristic shift vectors are presented in Table 1.

Projections of reducible space groups onto rod groups

Up to orthorhombic systems, these projections are symmorphic rod groups. This can be explained very briefly. With the exception of the rhombohedral lattice, the centering vectors in three dimensions always have the component $\mathbf{c}/2$ and the projection $T^0_{G2} = \not{p}_{\mathbf{c}/2} = T(\mathbf{c}/2)$ of T_G onto $V(\mathbf{c})$ is generated by $\mathbf{c}/2$. The screw and glide translations $\mathbf{c}/2$ become elements of this group and hence all rod groups resulting from the projection of monoclinic and orthorhombic groups are symmorphic. The fourfold screw axis (sub1 or equivalently sub3), where the screw translation is $\mathbf{c}/4$ (and, equivalently, $3\mathbf{c}/4$), creates a fourfold screw axis (sub2) with respect to the translation subgroup $\not{p}_{\mathbf{c}/2}$. Analogously, the diamond plane creates an axial glide plane c.

The fourfold axes 4_1 and 4_3 always appear in pairs and 4_1 in Hermann–Mauguin symbols of I-centered space groups can be replaced by 4_3 without violating the logical origin of the symbol. With each threefold axis of a trigonal group are associated another two threefold screw axes of opposite chirality; the projection of T_G onto $V(\mathbf{c})$ is the group $T^0_{G2} = \not{p}_{\mathbf{c}/3} = T(\mathbf{c}/3)$ and the screw translations are multiples of $\mathbf{c}/3$, so that the projection results in an ordinary threefold axis. For groups C^6_{3v} and D^6_{3d}, an axial plane with glide translation $\mathbf{c}/2$ is present. Since 2 and 3 have no common divisor, the glide translation $\mathbf{c}/6$ occurs and the glide plane persits in the projection.

Projections of reducible space groups onto layer groups

Monoclinic systems. Each of the five monoclinic space-group types is presented in *International Tables for Crystallography* (1987) with three diagrams. The orthogonal projection leads to layer groups of an oblique system, the other two diagrams can be interpreted as skew projections that lead to layer groups of a rectangular system. The three types of cell choice with respect to the unique axis c are described by the Bravais letters A, B and I. The skew projections for the I case are, however, not explicitly presented. As a result, the diagrams that correspond to entries $I121$ and $I211$, $I1m1$ and $Im11$, $I1c1$ and $Ic11$; $I1a1$ and $Ib11$, $I12/m1$ and $I2/m11$, $I12/c1$ and $I2/c11$; $I12/a1$ and $I2/b11$ are missing even in the 1987 edition of *International Tables for Crystallography.* We conventionally consider the plane of the diagram as $E(\mathbf{a}, \mathbf{b})$, so that the two rectangular diagrams (lower and right) correspond to the choices $\mathbf{a}$ and $\mathbf{b}$ of unique axes. If the oblique diagram (c axis) shows the setting A (setting B from the other side), then the lower diagram corresponds to the setting C (viewed from both sides), which leads to Z decomposition and hence all these cases were already listed in paper I of this series. The diagrams on the right then correspond to settings A and B. If the oblique diagram corresponds to the setting I, then both side diagrams (lower and right) also correspond to the setting I. These are the missing diagrams. We list in Tables 2 and 3 the settings in small groups as they correspond to the choice of unique axes $\mathbf{c}$, $\mathbf{b}$ and $\mathbf{a}$. Oblique diagrams are therefore listed first. When a glide plane is present, we have two distinct group settings for the I setting of the lattice (four settings instead of three). The corresponding layer groups are monoclinic–oblique, the rod groups are monoclinic–orthogonal. This exhausts the cases with unique axis c.

Next there follows either two couples or two triplets of settings with unique axes b and a. Accordingly, there are settings A or I and B or I and for I settings there are still two distinct settings of groups with a glide plane. The resulting layer groups are monoclinic–rectangular; the rod groups are monoclinic–

Table 2. *Homomorphisms of reducible space groups onto layer and rod groups with respect to Z reductions: monoclinic groups*

			$\sigma_{\mathbf{ab}}$	$\sigma_{\mathbf{c}}$	$\mathbf{q}$
C_2	C_2^3	$A112$	$p_{\mathbf{b}/2}112$	$\not{p}_{\mathbf{c}/2}112$	$0, \mathbf{b}/4$
		$B112$	$p_{\mathbf{a}/2}112$	$\not{p}_{\mathbf{c}/2}112$	$0, \mathbf{a}/4$
		$I112$	$\hat{p}112$	$\not{p}_{\mathbf{c}/2}112$	$0, (\mathbf{a}+\mathbf{b})/4$
		$A121$	$p_{\mathbf{b}/2}121$	$\not{p}_{\mathbf{c}/2}121$	$0, \mathbf{c}/4$
		$I121$	$c121$	$\not{p}_{\mathbf{c}/2}121$	$0, \mathbf{c}/4$
		$B211$	$p_{\mathbf{a}/2}211$	$\not{p}_{\mathbf{c}/2}211$	$0, \mathbf{c}/4$
		$I211$	$c211$	$\not{p}_{\mathbf{c}/2}211$	$0, \mathbf{c}/4$
C_s	C_s^3	$A11m$	$p_{\mathbf{b}/2}11\mathbf{m}$	$\not{p}_{\mathbf{c}/2}11m$	$0, \mathbf{c}/4$
		$B11m$	$p_{\mathbf{a}/2}11\mathbf{m}$	$\not{p}_{\mathbf{c}/2}11m$	$0, \mathbf{c}/4$
		$I11m$	$\hat{p}11m$	$\not{p}_{\mathbf{c}/2}11m$	$0, \mathbf{c}/4$
		$A1m1$	$P_{\mathbf{b}/2}1m1$	$\not{p}_{\mathbf{c}/2}1m1$	$0, \mathbf{b}/4$
		$I1m1$	$c1m1$	$\not{p}_{\mathbf{c}/2}1m1$	0
		$Bm11$	$p_{\mathbf{a}/2}m11$	$\not{p}_{\mathbf{c}/2}m11$	$0, \mathbf{a}/4$
		$Im11$	$cm11$	$\not{p}_{\mathbf{c}/2}m11$	0
	C_s^4	$A11a$	$p_{\mathbf{b}/2}11a$	$\not{p}_{\mathbf{c}/2}11m$	$0, \mathbf{c}/4$
		$B11b$	$p_{\mathbf{a}/2}11b$	$\not{p}_{\mathbf{c}/2}11m$	$0, \mathbf{c}/4$
		$I11a$	$\hat{p}11n$	$\not{p}_{\mathbf{c}/2}11m$	$0, \mathbf{c}/4$
		$I11b$	$\hat{p}11n$	$\not{p}_{\mathbf{c}/2}11m$	$0, \mathbf{c}/4$
		$A1a1$	$p_{\mathbf{b}/2}1a1$	$\not{p}_{\mathbf{c}/2}1m1$	$0, \mathbf{b}/4$
		$I1c1$	$c1m1$	$\not{p}_{\mathbf{c}/2}1m1$	0
		$I1a1$	$c1m1$	$\not{p}_{\mathbf{c}/2}1m1$	0
		$Bb11$	$p_{\mathbf{a}/2}b11$	$\not{p}_{\mathbf{c}/2}m11$	$0, \mathbf{a}/4$
		$Ic11$	$cm11$	$\not{p}_{\mathbf{c}/2}m11$	0
		$Ib11$	$cm11$	$\not{p}_{\mathbf{c}/2}m11$	0
C_{2h}	C_{2h}^3	$A112/m$	$p_{\mathbf{b}/2}112/m$	$\not{p}_{\mathbf{c}/2}112/m$	$0, \mathbf{b}/4, \mathbf{c}/4, (\mathbf{b}+\mathbf{c})/4$
		$B112/m$	$p_{\mathbf{a}/2}112/m$	$p_{\mathbf{c}/2}112/m$	$0, \mathbf{a}/4, \mathbf{c}/4, (\mathbf{a}+\mathbf{c})/4$
		$I112/m$	$\hat{p}112/m$	$\not{p}_{\mathbf{c}/2}112/m$	$0, (\mathbf{a}+\mathbf{b})/4, \mathbf{c}/4, (\mathbf{a}+\mathbf{b}+\mathbf{c})/4$
		$A12/m1$	$p_{\mathbf{b}/2}12/m1$	$\not{p}_{\mathbf{c}/2}12/m1$	$0, \mathbf{b}/4, \mathbf{c}/4, (\mathbf{b}+\mathbf{c})/4$
		$I12/m1$	$c12/m1$	$\not{p}_{\mathbf{c}/2}12/m1$	$0, \mathbf{c}/4$
		$B2/m11$	$p_{\mathbf{a}/2}2/m11$	$\not{p}_{\mathbf{c}/2}2/m11$	$0, \mathbf{a}/4, \mathbf{c}/4, (\mathbf{a}+\mathbf{c})/4$
		$I2/m11$	$c2/m11$	$\not{p}_{\mathbf{c}/2}2/m11$	$0, \mathbf{c}/4$
	C_{2h}^5	$A112/a$	$p_{\mathbf{b}/2}112/a$	$\not{p}_{\mathbf{c}/2}112/m$	$0, \mathbf{b}/4, \mathbf{c}/4, (\mathbf{b}+\mathbf{c})/4$
		$B112/b$	$p_{\mathbf{a}/2}112/b$	$\not{p}_{\mathbf{c}/2}112/m$	$0, \mathbf{a}/4, \mathbf{c}/4, (\mathbf{a}+\mathbf{c})/4$
		$I112/b$	$\hat{p}112/n$	$\not{p}_{\mathbf{c}/2}112/m$	$0, (\mathbf{a}+\mathbf{b})/4, \mathbf{c}/4, (\mathbf{a}+\mathbf{b}+\mathbf{c})/4$
		$I112/a$	$\hat{p}112/n$	$\not{p}_{\mathbf{c}/2}112/m$	$0, (\mathbf{a}+\mathbf{b})/4, \mathbf{c}/4, (\mathbf{a}+\mathbf{b}+\mathbf{c})/4$
		$A12/a1$	$p_{\mathbf{b}/2}12/a$	$\not{p}_{\mathbf{c}/2}1212/m1$	$0, \mathbf{b}/4, \mathbf{c}/4, (\mathbf{b}+\mathbf{c})/4$
		$I12/c1$	$c12/m1$	$\not{p}_{\mathbf{c}/2}12/m1$	$0, \mathbf{c}/4$
		$I12/a1$	$c12/m1$	$\not{p}_{\mathbf{c}/2}12/m1$	$0, \mathbf{c}/4$
		$B2/b11$	$p_{\mathbf{a}/2}2/b11$	$\not{p}_{\mathbf{c}/2}2/m11$	$0, \mathbf{a}/4, \mathbf{c}/4, (\mathbf{a}+\mathbf{c})/4$
		$I2/c11$	$c2/m11$	$\not{p}_{\mathbf{c}/2}2/m11$	$0, \mathbf{c}/4$
		$I2/b11$	$c2/m11$	$\not{p}_{\mathbf{c}/2}2/m11$	$0, \mathbf{c}/4$

inclined. The treatment of diagrams is analogous to the corresponding cases of *A*, *B* and *I* centerings of orthorhombic groups.

Orthorhombic systems. Since the *A* and *B* centerings correspond to two views of the same diagram, it is sufficient to consider only one of these centerings, say the *A* centering.

A centering. The coupling of the centering vector $(\mathbf{b}+\mathbf{c})/2$ with an inversion center or a twofold *a* axis generates the same kind of element at a distance $(\mathbf{b}+\mathbf{c})/4$. The mirror *b* plane is associated with an axial *b* plane $(\mathbf{c}/2)$ and an axial *b* plane $(\mathbf{a}/2)$ is associated with a diagonal *b* plane $[(\mathbf{a}+\mathbf{c})/2]$. The glide translation $\mathbf{c}/2$ is lost on projection so the partners project onto the same kind of element of a layer group - a mirror plane and an axial plane $(\mathbf{a}/2)$, respectively. The twofold *b* axis is associated with a twofold screw axis at a distance $\mathbf{c}/4$ with a screw translation $\mathbf{b}/2$. The latter is, however, an element of T^0_{G1} and hence both axes project as an ordinary twofold axis. The twofold *c* axis is accompanied by a twofold screw axis at a distance $\mathbf{b}/4$ that loses its screw translation $\mathbf{c}/2$ in the projection. The mirror *c* plane creates an axial plane $(\mathbf{b}/2)$ at a distance $\mathbf{c}/4$ and, since $\mathbf{b}/2$ belongs to T^0_{G1}, both planes project to an ordinary mirror plane - the plane of the layer group. The axial *c* plane $(\mathbf{a}/2)$ associates with the diagonal one $[(\mathbf{a}+\mathbf{b})/2]$ and both project again to an axial *c* plane $(\mathbf{a}/2)$. The *a* planes are a special case. Since the centering vector $(\mathbf{b}+\mathbf{c})/2$ lies in a plane, the mirror *a* plane is simultaneously a diagonal *a* plane $[(\mathbf{b}+\mathbf{c})/2]$ and the axial *a* plane $(\mathbf{b}/2)$ is simultaneously an axial *a* plane $(\mathbf{c}/2)$. In other words, the full line is equivalent to a dash-dotted line; the dashed is equivalent to dotted. In Hermann-Mauguin symbols we can use interchangeably the letters *m*, *n* for the first of these planes, *b*, *c* for the second (*a* and *c* in the *B* setting). The reader can check the use of alternative diagrams and symbols for groups C^{14}_{2v}: $Amm2$ ($Anm2$), $Am2m$ ($An2m$) or $Bmm2$ ($Bmn2$), $B2mm$ ($B2nm$); C^{15}_{2v}: $Abm2$ ($Acm2$), $Ac2m$ ($Ab2m$) or $Bma2$ ($Bmc2$), $B2cm$ ($B2am$) and analogously for

Table 3. *Homomorphisms of reducible space groups onto layer and rod groups with respect to Z reductions: orthorhombic groups*

			σ_{ab}	σ_c	q
D_2	D_2^5	$B22_12$	$p_{a/2}22_12$	$\not{p}_{c/2}222$	0, a/4, c/4, (a+c)/4
		$A2_122$	$p_{b/2}2_122$	$\not{p}_{c/2}222$	0, b/4, c/4, (b+c)/4
	D_2^6	$B222$	$p_{a/2}222$	$\not{p}_{c/2}222$	0, a/4, c/4, (a+c)/4
		$A222$	$p_{b/2}222$	$\not{p}_{c/2}222$	0, b/4, c/4, (b+c)/4
	D_2^7	$F222$	$p_{a/2,b/2}222$	$\not{p}_{c/2}222$	0, a/4, b/4, c/4, (a+b)/4, (b+c)/4, (c+a)/4, (a+b+c)/4
	D_2^8	$I222$	$c222$	$\not{p}_{c/2}222$	0
	D_2^9	$I2_12_12_1$	$c222$	$\not{p}_{c/2}222$	0
C_{2v}	C_{2v}^{11}	$Bm2m$	$p_{a/2}m2m$	$\not{p}_{c/2}m2m$	0, a/4, c/4, (a+c)/4
		$A2mm$	$p_{b/2}2mm$	$\not{p}_{c/2}2mm$	0, b/4, c/4, (b+c)/4
	C_{2v}^{12}	$Bm2_1b$	$p_{a/2}m2_1b$	$\not{p}_{c/2}m2m$	0, a/4, c/4, (a+c)/4
		$A2_1ma$	$p_{b/2}2_1ma$	$\not{p}_{c/2}2mm$	0, b/4, c/4, (b+c)/4
		$Bb2_1m$	$p_{a/2}b2_1m$	$\not{p}_{c/2}m2m$	0, a/4, c/4, (a+c)/4
		$A2_1am$	$p_{b/2}2_1am$	$\not{p}_{c/2}2mm$	0, b/4, c/4, (b+c)/4
	C_{2v}^{13}	$Bb2b$	$p_{a/2}b2b$	$\not{p}_{c/2}m2m$	0, a/4, c/4, (a+c)/4
		$A2aa$	$p_{b/2}2aa$	$\not{p}_{c/2}2mm$	0, b/4, c/4, (b+c)/4
	C_{2v}^{14}	$Amm2$	$p_{b/2}mm2$	$\not{p}_{c/2}mm2$	0, b/4
		$Bmm2$	$p_{a/2}mm2$	$\not{p}_{c/2}mm2$	0, a/4
		$Am2m$	$p_{b/2}m2m$	$\not{p}_{c/2}m2m$	0, c/4
		$B2mm$	$p_{a/2}2mm$	$\not{p}_{c/2}2mm$	0, c/4
	C_{2v}^{15}	$Abm2$	$p_{b/2}bm2$	$\not{p}_{c/2}mm2$	0, b/4
		$Bma2$	$p_{a/2}ma2$	$\not{p}_{c/2}mm2$	0, a/4
		$Ac2m$	$p_{b/2}m2m$	$\not{p}_{c/2}m2m$	0, c/4
		$B2cm$	$p_{a/2}2mm$	$\not{p}_{c/2}2mm$	0, c/4
	C_{2v}^{16}	$Ama2$	$p_{b/2}ma2$	$\not{p}_{c/2}mm2$	0, b/4
		$Bbm2$	$p_{a/2}bm2$	$\not{p}_{c/2}mm2$	0, a/4
		$Am2a$	$p_{b/2}m2a$	$\not{p}_{c/2}m2m$	0, c/4
		$B2mb$	$p_{a/2}2mb$	$\not{p}_{c/2}2mm$	0, c/4
	C_{2v}^{17}	$Aba2$	$p_{b/2}ma2$	$\not{p}_{c/2}mm2$	0, b/4
		$Bba2$	$p_{a/2}bm2$	$\not{p}_{c/2}mm2$	0, a/4
		$Ac2a$	$p_{b/2}m2a$	$\not{p}_{c/2}m2m$	0, c/4
		$B2cb$	$p_{a/2}2mb$	$\not{p}_{c/2}2mm$	0, c/4
C_{2v}	C_{2v}^{18}	$Fmm2$	$p_{a/2,b/2}mm2$	$\not{p}_{c/2}mm2$	0, a/4, b/4, (a+b)/4
		$Fm2m$	$p_{a/2,b/2}m2m$	$\not{p}_{c/2}m2m$	0, a/4, c/4, (a+c)/4
		$F2mm$	$p_{a/2,b/2}2mm$	$\not{p}_{c/2}2mm$	0, b/4, c/4, (b+c)/4
	C_{2v}^{19}	$Fdd2$	$p_{a/2,b/2}ba2$	$\not{p}_{c/2}mm2$	0, a/4, b/4, (a+b)/4
		$Fd2d$	$p_{a/2,b/2}b2n$	$\not{p}_{c/2}m2m$	0, a/4, c/4, (a+c)/4
		$F2dd$	$p_{a/2,b/2}2an$	$\not{p}_{c/2}2mm$	0, b/4, c/4, (b+c)/4
	C_{2v}^{20}	$Imm2$	$cmm2$	$\not{p}_{c/2}mm2$	0
		$Im2m$	$cm2m$	$\not{p}_{c/2}m2m$	0, c/4
		$I2mm$	$c2mm$	$\not{p}_{c/2}2mm$	0, c/4
	C_{2v}^{21}	$Iba2$	$cmm2$	$\not{p}_{c/2}mm2$	0
		$Ic2a$	$cm2a$	$\not{p}_{c/2}m2m$	0, c/4
		$I2cb$	$c2mb$	$\not{p}_{c/2}2mm$	0, c/4
	C_{2v}^{22}	$Ima2$	$cmm2$	$\not{p}_{c/2}mm2$	0
		$Ibm2$	$cmm2$	$\not{p}_{c/2}mm2$	0
		$Im2a$	$cm2a$	$\not{p}_{c/2}m2m$	0, c/4
		$I2mb$	$c2mb$	$\not{p}_{c/2}2mm$	0, c/4
		$I2cm$	$c2mm$	$\not{p}_{c/2}2mm$	0, c/4
		$Ic2m$	$cm2m$	$\not{p}_{c/2}m2m$	0, c/4
D_{2h}	D_{2h}^{17}	$Bmmb$	$p_{a/2}mmb$	$\not{p}_{c/2}mmm$	0, a/4, c/4, (a+c)/4
		$Amma$	$p_{b/2}mma$	$\not{p}_{c/2}mmm$	0, b/4, c/4, (b+c)/4
		Ama	$p_{b/2}mam$	$\not{p}_{c/2}mmm$	0, b/4, c/4, (b+c)/4
		$Bbmm$	$p_{a/2}bmm$	$\not{p}_{c/2}mmm$	0, a/4, c/4, (a+c)/4
	D_{2h}^{18}	$Bmam$	$p_{a/2}mab$	$\not{p}_{c/2}mmm$	0, a/4, c/4, (a+c)/4
		$Abma$	$p_{b/2}bma$	$\not{p}_{c/2}mmm$	0, b/4, c/4, (b+c)/4
		$Acam$	$p_{b/2}mam$	$\not{p}_{c/2}mmm$	0, b/4, c/4, (b+c)/4
		$Bbcm$	$p_{a/2}bmm$	$\not{p}_{c/2}mmm$	0, a/4, c/4, (a+c)/4
	D_{2h}^{19}	$Bmmm$	$p_{a/2}mmm$	$\not{p}_{c/2}mmm$	0, a/4, c/4, (a+c)/4
		$Ammm$	$p_{b/2}mmm$	$\not{p}_{c/2}mmm$	0, b/4, c/4, (b+c)/4
	D_{2h}^{20}	$Bbmb$	$p_{a/2}bmb$	$\not{p}_{c/2}mmm$	0, a/4, c/4, (a+c)/4
		$Amaa$	$p_{b/2}maa$	$\not{p}_{c/2}mmm$	0, b/4, c/4, (b+c)/4
	D_{2h}^{21}	$Bmam$	$p_{a/2}mmm$	$\not{p}_{c/2}mmm$	0, a/4, c/4, (a+c)/4
		$Abmm$	$p_{b/2}mmm$	$\not{p}_{c/2}mmm$	0, b/4, c/4, (b+c)/4
		$Acmm$	$p_{b/2}mmm$	$\not{p}_{c/2}mmm$	0, b/4, c/4, (b+c)/4
		$Bmcm$	$p_{a/2}mmm$	$\not{p}_{c/2}mmm$	0, a/4, c/4, (a+c)/4
	D_{2h}^{22}	$Bbab$	$p_{a/2}bab$	$\not{p}_{c/2}mmm$	0, a/4, c/4, (a+c)/4
		$Abaa$	$p_{b/2}baa$	$\not{p}_{c/2}mmm$	0, b/4, c/4, (b+c)/4
		$Acaa$	$p_{b/2}maa$	$\not{p}_{c/2}mmm$	0, b/4, c/4, (b+c)/4
		$Bbcb$	$p_{a/2}bmb$	$\not{p}_{c/2}mmm$	0, a/4, c/4, (a+c)/4

Table 3 (*cont.*)

			$\sigma_{\mathbf{ab}}$	$\sigma_{\mathbf{c}}$	$\mathbf{q}$
D_{2h}	D_{2h}^{23}	*Fmmm*	$p_{\mathbf{a}/2,\mathbf{b}/2}mmm$	$\not{p}_{\mathbf{c}/2}mmm$	$\mathbf{0}$, $\mathbf{a}/4$, $\mathbf{b}/4$, $\mathbf{c}/4$, $(\mathbf{a}+\mathbf{b})/4$, $(\mathbf{b}+\mathbf{c})/4$, $(\mathbf{c}+\mathbf{a})/4$, $(\mathbf{a}+\mathbf{b}+\mathbf{c})/4$
	D_{2h}^{24}	*Fddd*	$p_{\mathbf{a}/2,\mathbf{b}/2}ban$	$\not{p}_{\mathbf{c}/2}mmm$	$\mathbf{0}$, $\mathbf{a}/4$, $\mathbf{b}/4$, $\mathbf{c}/4$, $(\mathbf{a}+\mathbf{b})/4$, $(\mathbf{b}+\mathbf{c})/4$, $(\mathbf{c}+\mathbf{a})/4$, $(\mathbf{a}+\mathbf{b}+\mathbf{c})/4$
	D_{2h}^{25}	*Immm*	*cmmm*	$\not{p}_{\mathbf{c}/2}mmm$	$\mathbf{0}$, $\mathbf{c}/4$
	D_{2h}^{26}	*Ibam*	*cmmm*	$\not{p}_{\mathbf{c}/2}mmm$	$\mathbf{0}$, $\mathbf{c}/4$
		Icma	*cmma*(*b*)	$\not{p}_{\mathbf{c}/2}mmm$	$\mathbf{0}$, $\mathbf{c}/4$
		Imcb	*cmma*(*b*)	$\not{p}_{\mathbf{c}/2}mmm$	$\mathbf{0}$, $\mathbf{c}/4$
	D_{2h}^{27}	*Ibcc*	*cmma*(*b*)	$\not{p}_{\mathbf{c}/2}mmm$	$\mathbf{0}$, $\mathbf{c}/4$
	D_{2h}^{28}	*Imma*	*cmma*(*b*)	$\not{p}_{\mathbf{c}/2}mmm$	$\mathbf{0}$, $\mathbf{c}/4$
		Immb	*cmma*(*b*)	$\not{p}_{\mathbf{c}/2}mmm$	$\mathbf{0}$, $\mathbf{c}/4$
		Imam	*cmmm*	$\not{p}_{\mathbf{c}/2}mmm$	$\mathbf{0}$, $\mathbf{c}/4$
		Ibmm	*cmmm*	$\not{p}_{\mathbf{c}/2}mmm$	$\mathbf{0}$, $\mathbf{c}/4$
		Icmm	*cmmm*	$\not{p}_{\mathbf{c}/2}mmm$	$\mathbf{0}$, $\mathbf{c}/4$
		Imcm	*cmm*	$\not{p}_{\mathbf{c}/2}mmm$	$\mathbf{0}$, $\mathbf{c}/4$

C_{2v}^{16}, C_{2v}^{17}: D_{2h}^{17}, D_{2h}^{18}, D_{2h}^{19}, D_{2h}^{20}. For groups D_{2h}^{21} and D_{2h}^{22} pairs of different symbols and diagrams are used for otherwise evidently identical settings of the same space groups [*Bmam* = *Bmcm*, *Abmm* = *Acmm* for D_{2h}^{21} and *Bbab* = *Bbcb*, *Abaa* = *Acaa* for D_{2h}^{22}]. In the first case, the groups differ by the origin choice, in the second they are completely identical.

F centering. There are three centering vectors $(\mathbf{b}+\mathbf{c})/2$, $(\mathbf{a}+\mathbf{c})/2$ and $(\mathbf{a}+\mathbf{b})/2$, of which the last lies in the plane of the layer group. The translation subgroup of the layer groups is, however, generated by vectors $\mathbf{a}/2$ and $\mathbf{b}/2$. It is easy to see that one inversion center is associated with another three and a twofold axis with another and in addition two screw axes. A mirror plane is at the same time a diagonal one and has a partner that is axial in two directions. All these elements project as symmorphic ones. The diamond planes appear in pairs and project as diagonal planes.

I centering. The coupling of elements with the centering vector $(\mathbf{a}+\mathbf{b}+\mathbf{c})/2$ associates a twofold screw axis with the ordinary axis. For *c* axes, both project as ordinary axes but for axes parallel with the diagram the screw axes again project as screw axes. The mirror plane associates with a diagonal plane and two axial planes are always associated with glide translations in perpendicular directions. The planes perpendicular to the diagram project as usual in *P* cases. The pair consisting of a mirror plane and diagonal plane parallel with the plane of the diagram projects as the plane of the layer group, while the two planes with perpendicular glide translations project onto a layer plane with two axial glide translations. The lattice of the layer group is of the *c* type here, which just allows such a symmetry element. All projections obtained by this analysis of orthorhombic groups are given in Table 3.

Tetragonal system. The projection of the *I* lattice with the centering vector $(\mathbf{a}+\mathbf{b}+\mathbf{c})/2$ results in a square lattice $\hat{p}$ with bases $(\mathbf{a}+\mathbf{b})/2$, $(\mathbf{a}-\mathbf{b})/2$. The centering vector couples with inversion centers, twofold axes and planes in the same way as for orthorhombic *I*-centered cases. In particular, the diamond planes project onto axial planes as we can see by comparison of the projections $(\mathbf{a}+\mathbf{b})/4$ of the diamond glide translation $(\mathbf{a}\pm\mathbf{b}-\mathbf{c})/4$ with basis vectors $(\mathbf{a}\pm\mathbf{b})/2$. All fourfold axes project to ordinary ones. The projections are listed in Table 4.

Table 4. *Homomorphisms of reducible space groups onto layer and rod groups with respect to Z reductions: tetragonal groups*

			$\sigma_{\mathbf{ab}}$	$\sigma_{\mathbf{c}}$	$\mathbf{q}$
C_4	C_4^5	$I4$	$p4$	$\not{p}_{\mathbf{c}/2}4$	$\mathbf{0}$, $\mathbf{a}/2$
	C_4^6	$I4_1$	$p4$	$\not{p}_{\mathbf{c}/2}4_2$	$\mathbf{0}$, $\mathbf{a}/2$
S_4	S_4^2	$I\bar{4}$	$p\bar{4}$	$\not{p}_{\mathbf{c}/2}\bar{4}$	$\mathbf{0}$, $\mathbf{c}/4$
C_{4h}	C_{4h}^5	$I4/m$	$p4/m$	$\not{p}_{\mathbf{c}/2}4/m$	$\mathbf{0}$, $\mathbf{a}/2$, $\mathbf{c}/4$, $\mathbf{a}/2+\mathbf{c}/4$
	C_{4h}^6	$I4_1/a$	$p4/m$	$\not{p}_{\mathbf{c}/2}4_2/m$	$\mathbf{0}$, $\mathbf{a}/2$, $\mathbf{c}/4$, $\mathbf{a}/2+\mathbf{c}/4$
D_4	D_4^9	$I422$	$p422$	$\not{p}_{\mathbf{c}/2}422$	$\mathbf{0}$, $\mathbf{a}/2$, $\mathbf{c}/4$, $\mathbf{a}/2+\mathbf{c}/4$
	D_4^{10}	$I4_122$	$p422$	$\not{p}_{\mathbf{c}/2}4_222$	$\mathbf{0}$, $\mathbf{a}/2$, $\mathbf{c}/4$, $\mathbf{a}/2+\mathbf{c}/4$
C_{4v}	C_{4v}^9	$I4mm$	$p4mm$	$\not{p}_{\mathbf{c}/2}4mm$	$\mathbf{0}$, $\mathbf{a}/2$
	C_{4v}^{10}	$I4cm$	$p4mm$	$\not{p}_{\mathbf{c}/2}4mm$	$\mathbf{0}$, $\mathbf{a}/2$
	C_{4v}^{11}	$I4_1cd$	$p4bm$	$\not{p}_{\mathbf{c}/2}4_2cm$	$\mathbf{0}$, $\mathbf{a}/2$
	C_{4v}^{12}	$I4_1md$	$p4bm$	$\not{p}_{\mathbf{c}/2}4_2cm$	$\mathbf{0}$, $\mathbf{a}/2$
D_{2d}	D_{2d}^9	$I\bar{4}m2$	$p\bar{4}2m$	$\not{p}_{\mathbf{c}/2}\bar{4}m2$	$\mathbf{0}$, $\mathbf{c}/4$
	D_{2d}^{10}	$I\bar{4}c2$	$p\bar{4}2m$	$\not{p}_{\mathbf{c}/2}\bar{4}c2$	$\mathbf{0}$, $\mathbf{c}/4$
	D_{2d}^{11}	$I\bar{4}2m$	$p\bar{4}m2$	$\not{p}_{\mathbf{c}/2}\bar{4}2m$	$\mathbf{0}$, $\mathbf{c}/4$
	D_{2d}^{12}	$I\bar{4}2d$	$p\bar{4}b2$	$\not{p}_{\mathbf{c}/2}\bar{4}2m$	$\mathbf{0}$, $\mathbf{c}/4$
D_{4h}	D_{4h}^{17}	$I4/mmm$	$p4/mmm$	$\not{p}_{\mathbf{c}/2}4/mmm$	$\mathbf{0}$, $\mathbf{a}/2$, $\mathbf{c}/4$, $\mathbf{a}/2+\mathbf{c}/4$
	D_{4h}^{18}	$I4/mcm$	$p4/mmm$	$\not{p}_{\mathbf{c}/2}4/mmm$	$\mathbf{0}$, $\mathbf{a}/2$, $\mathbf{c}/4$, $\mathbf{a}/2+\mathbf{c}/4$
	D_{4h}^{19}	$I41/amd$	$p4/nbm$	$\not{p}_{\mathbf{c}/2}4_2/mmc$	$\mathbf{0}$, $\mathbf{a}/2$, $\mathbf{c}/4$, $\mathbf{a}/2+\mathbf{c}/4$
	D_{4h}^{20}	$I41/acd$	$p4/nbm$	$\not{p}_{\mathbf{c}/2}4_2/mmc$	$\mathbf{0}$, $\mathbf{a}/2$, $\mathbf{c}/4$, $\mathbf{a}/2+\mathbf{c}/4$

Trigonal system. The rhombohedral translation groups are subdirect sums of either of the following forms:

$$T(\mathbf{a}, \mathbf{b}) \oplus T(\mathbf{c})[\mathbf{0} \cup (2\mathbf{a}+\mathbf{b}+\mathbf{c})/3 \cup (\mathbf{a}+2\mathbf{b}+2\mathbf{c})/3],$$

$$T(\mathbf{a}, \mathbf{b}) \oplus T(\mathbf{c})[\mathbf{0} \cup (\mathbf{a}+2\mathbf{b}+\mathbf{c})/3 \cup (2\mathbf{a}+\mathbf{b}+2\mathbf{c})/3],$$

where $T(\mathbf{a}, \mathbf{b}) \oplus T(\mathbf{c}) = T_{G1} \oplus T_{G2} = T_{G0}$ is the translation group that corresponds to the hexagonal primitive lattice. The subdirect summands are in both cases the groups: $T_{G1}^0 = \hat{p}_{1/3} = T[(2\mathbf{a}+\mathbf{b})/3, (\mathbf{a}+2\mathbf{b})/3]$ and $T_{G_2}^0 = \not{p}_{1/3} = T(\mathbf{c}/3)$ (see paper I or Kopský, 1988). Accordingly, there exist two possible settings with respect to the conventional hexagonal basis $(\mathbf{a}, \mathbf{b}, \mathbf{c})$: the obverse setting, used in the 1987 edition of *Inter-*

Table 5. *Homomorphisms of reducible space groups onto layer and rod groups with respect to Z reductions: trigonal groups*

			σ_{ab}	σ_c	q
C_3	C_3^4	$R3$	$\hat{p}_{1/3}3$	$\not{p}_{c/3}3$	0, a/3, 2a/3
C_{3i}	C_{3i}^2	$R\bar{3}$	$\hat{p}_{1/3}\bar{3}$	$\not{p}_{c/3}\bar{3}$	0, c/6, c/3
D_3	D_3^7	$R32$	$\hat{p}_{1/3}312$	$\not{p}_{c/3}321$	0, a/3, 2a/3, c/6, c/3, a/3+c/6, a/3+c/3, 2a/3+c/6, 2a/3+c/3
C_{3v}	C_{3v}^5	$R3m$	$\hat{p}_{1/3}31m$	$\not{p}_{c/3}3m1$	0, a/3, 2a/3
	C_{3v}^6	$R3c$	$\hat{p}_{1/2}31m$	$\not{p}_{c/3}3c1$	
D_{3d}	D_{3d}^5	$R\bar{3}m$	$\hat{p}_{1/3}\bar{3}12/m$	$\not{p}_{c/3}\bar{3}m1$	0, a/3, 2a/3, c/6, c/3, a/3+c/6, a/3+c/3, 2a/3+c/6, 2a/3+c/3
	D_{3d}^6	$R\bar{3}c$	$\hat{p}_{1/3}\bar{3}12/m$	$\not{p}_{c/3}\bar{3}c1$	

national Tables for Crystallography as well as in the 1952/1969 editions of *International Tables for X-ray Crystallography*; and the reverse setting used in the first edition of Vol. I of *Internationalle Tabellen zur Bestimmung von Kristallstrukturen* (1935). The rotation of a group by $\pi/3$ around the hexagonal axis sends it from one setting to the other. It leaves both homomorphic projections (layer and rod groups) invariant, so that they are the same for both obverse and inverse settings. They are listed in Table 5.

7. Concluding remarks

Let us briefly overview what we have described in the two papers and what still should be done. We have determined homomorphic projections of reducible plane and space groups onto their factor groups with respect to all types of Z reductions and Z decompositions. The projections connected with Z decompositions were used to introduce the nomenclature and symbols of frieze, layer and rod groups compatible with symbols for plane and space groups. The determination of factor groups is also equivalent to the classification of reducible plane and space groups into pairs of frieze-group classes and into pairs of layer- and rod-group classes, respectively. We must say, however, that this is not the end of the problem up to three dimensions. An exact and complete solution must also involve the problem of origin choices since there are cases where we may list a layer or rod group as a projection of different space groups using the same symbol for this layer and/or rod group, even though these projections have different locations in space, if we accept that the location of the space group is given by its diagram. There is only one remedy for this: we have to fix the Hermann–Mauguin symbols of space groups and of frieze, layer and rod groups to certain standard origin choices and use modified symbols if the groups are shifted in space. The addition to the standard symbol of a shift vector in parentheses would give a simple and clear convention for this purpose.

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Automatic Determination of Crystal Structures using Karle–Hauptman Matrices

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Abstract

This paper describes a method for automatic structure determination by the application of Karle–Hauptman matrices to the phase problem. A new method, the common-minor strategy, is used to combine the information contained in several Karle–Hauptman matrices. Sets of phases large enough to define the

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