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Layer and Rod Classes of Reducible Space Groups. I. Z-Decomposable Cases

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Abstract

Reducible plane groups are classified into pairs of frieze-group classes; reducible space groups are classified into pairs of layer and rod classes with respect to all possible Z decompositions. Firstly, all reductions of translation groups to the form of a direct sum (Z decomposition) or of a subdirect sum (Z) reduction) of two G-invariant translation groups of lower dimensions are determined according to Bravais types. A practical way to determine layer and rod classes with the use of standard space-group diagrams is described and a geometric interpretation of symmorphic representatives of these classes is explained. Tables of the distribution of plane groups into pairs of frieze classes and of space groups into layer and rod classes with respect to possible Zdecompositions are given. A notation for layer and rod groups compatible with Hermann-Mauguin symbols for space groups is used; compatibility is achieved on the basis of the factorization procedure.

1. Introduction

This is the first part of a two-paper series [paper II: Fuksa & Kopský (1993)] in which we apply the results of dimension-independent analysis of the factorization of reducible space groups by their partial translation subgroups (Kopský, 1989a, b) to plane groups and to space groups in three dimensions. We start with a brief review of the factorization procedure to make the reader familiar with symbols and terms used in the papers by Kopský (1989a, b), which will be referred to as papers A and B. According to the definition of a reducible space group, the plane groups of oblique and rectangular systems and all space groups, with the exception of cubic ones, are reducible. The translation subgroup T_G of a reducible space group G contains 'partial translation subgroups' that are maximal in the sense that they are equivalent to intersections of T_G with the rational (or real) space they themselves generate and invariant under the point group G and hence normal in G.

According to the 'factorization theorem' (paper A, theorem 2), the factor groups of reducible space groups over partial translation subgroups have the structure of subperiodic groups. The whole T_G is

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either a direct sum (Z decomposition) of complementary partial translation subgroups or it contains their direct sum as its proper subgroup of finite index (Z reduction). In both cases, we can assign the space group G to a pair of complementary classes of subperiodic groups with respect to a given Z decomposition or Z reduction.

Classification of reducible plane groups into pairs of frieze-group classes has already been considered by Litvin & Kopský (1987) and it is discussed here only for completeness. Reducible space groups are accordingly classified into pairs, consisting of a layer and of a rod class. We shall determine here all types of Z decompositions and of Z reductions for plane and space groups and perform classification for Z decompositions. Factorization for Z reductions has special features and will be considered in the next paper.

An actual factorization and hence the distribution of space groups into layer and rod classes is performed on the basis of space-group diagrams from *International Tables for Crystallography* (1987), referred to as *IT*87. It has been known for a long time (Cochran, 1952; Kathleen Lonsdale, personal communication) that for each layer group there exists a space group with the same diagram. We shall explain the group-theoretical nature of this relationship and show that an analogous relationship can be found for rod groups. The factorization procedure itself will be used to deduce the Hermann-Mauguin symbols for layer and rod groups, which are compatible with the notation for the space groups.

2. A brief review of the factorization procedure

A reducible space group $\mathbb{G} = \{G, T_G, P, \mathbf{u}_G(g)\}$ has the following property: the vector space V(n, R)splits, perhaps in several or even infinitely many ways. into G-invariant crystallographic subspaces $V_1(k, R)$ and $V_2(h, R)$, of which V(n, R) is a direct sum. The word 'crystallographic' means that the intersections $T_{G_1} = T_G \cap V_1(k, R)$ and $T_{G_2} = T_G \cap V_2(h, R)$ are partial translation subgroups that span the spaces $V_1(k, R)$ and $V_2(h, R)$, respectively. The reduction $V(n, R) = V_1(k, R) \oplus V_2(h, R)$ is the reduction in the field of real numbers or, in earlier nomenclature, an *R* reduction. If it is crystallographic, then it implies a Q reduction, the former name for the reduction of the rational space $V(T_G, Q)$, spanned by T_G , into a direct sum of G-invariant rational subspaces $V_1(T_G,$ Q) and $V_2(T_{G2}, Q)$. With each such R reduction we associate two homomorphisms: $\sigma_1: V(n, R) \rightarrow$ $V_1(k, R)$ and $\sigma_2: V(n, R) \rightarrow V_2(h, R)$, which can be interpreted as projections of vectors t from the space V(n, R) onto their components $\sigma_1(t) = t_1 = V_1(k, R)$ and $\sigma_2(\mathbf{t}) = \mathbf{t}_2 \in V_2(h, R)$ so that $\mathbf{t} = \mathbf{t}_1 + \mathbf{t}_2$.

The group T_G is then either a direct sum $T_{G1} \oplus T_{G2}$ of partial G-invariant translation subgroups $T_{G1} =$ $\sigma_1(T_G)$ and $T_{G2} = \sigma_2(T_G)$, which is a Z decomposition of the group T_G or it is expressed as

$$T_G = T_{G_1} \oplus T_{G_2} [\mathbf{0} \cup \mathbf{d}_2 \cup \ldots \cup \mathbf{d}_p]$$

which is the so-called Z reduction of T_G . In the latter case, the projections of the group T_G into the G-invariant subspaces are groups

$$\sigma_1(T_G) = T_{G_1}^0 = T_{G_1}[\mathbf{0} \cup \mathbf{d}_{21} \cup \ldots \cup \mathbf{d}_{p1}]$$

and

$$\sigma_2(T_G) = T_{G2}^0 = T_{G2}[\mathbf{0} \cup \mathbf{d}_{22} \cup \ldots \cup \mathbf{d}_{p2}],$$

of which T_G is a subdirect sum and the factor groups $T_G/(T_{G1} \oplus T_{G2})$, T_{G1}^0/T_{G1} and T_{G2}^0/T_{G2} are isomorphic (Kopský, 1988*a*).

Since they are G-invariant subgroups of T_G , the partial translation groups T_{G1} and T_{G2} are normal subgroups of G and, according to the factorization theorem (paper A, theorem 2), the factor groups \mathbb{G}/T_{G_1} and \mathbb{G}/T_{G_2} are isomorphic to subperiodic groups. The effect of various homomorphisms, connected with projection homomorphisms σ_1 and σ_2 has been analyzed (see paper A). The factor groups may be represented by so-called 'contracted subperiodic groups', which act on the Cartesian products $E_1(k) \times V_2(h, R)$ and $V_1(k, R) \times E_2(h)$ of the Euclidean spaces $E_1(k)$, $E_2(h)$, with their difference spaces, which are the subspaces $V_1(k, R)$ and $V_2(h, R)$; in both cases we combine the points of Euclidean space with vectors of complementary vector space.

The homomorphisms introduced by relations given in paper A, equation (10) then map the group G onto groups $\mathbb{L} = \sigma_1(\mathbb{G}) = [G, T_{G1}^0, P_1, \mathbf{u}_{G1}(g)] \simeq \mathbb{G}/T_{G2}$ and $\mathbb{R} = \sigma_2(\mathbb{G}) = \langle G, T_{G2}^0, P_2, \mathbf{u}_{G2}(g) \rangle \simeq \mathbb{G}/T_{G1}$, where $\mathbf{u}_{G1}(g) = \sigma_1[\mathbf{u}_G(g)], \mathbf{u}_{G2}(g) = \sigma_2[\mathbf{u}_G(g)]$ are projections of the system of nonprimitive translations $\mathbf{u}_G(g)$ onto G-invariant subspaces $V_1(k, R), V_2(h, R)$ and P_1, P_2 are the points of spaces $E_1(k), E_2(h)$ chosen as origins, corresponding to the origin P of E(n). Accordingly, we say that the space group G belongs to the pair of subperiodic classes \mathbb{L} and \mathbb{R} with respect to the reduction $V(n, R) = V_1(k, R) \oplus V_2(h, R)$.

3. Z decomposability and Z reducibility as properties of Bravais types

It is not necessary to consider the reduction scheme separately for each geometric class G. Indeed, each discrete translation group T has a particular holohedral symmetry G_0 and the pair (G_0, T) determines a particular Bravais arithmetic (Z) class; in other words, the Bravais type of T. Each arithmetic class (G, T) then belongs to a particular arithmetic Bravais class (Bülow, Neubüser & Wondratschek, 1971; Schwarzenberger, 1974). The assignment of arithmetic classes (G, T) to Bravais arithmetic classes (G_0, T) is such that, if there is no accidental degeneracy of the symmetry of T, the decomposition scheme is the same for G as for G_0 . The R and Qreductions are the properties of crystal families, while Z decompositions and reductions are the properties of Bravais flocks. The terminology used here follows that of Brown, Bülow, Neubüser, Wondratschek & Zassenhaus (1978) and the contribution by Wondratschek to *IT*87. Hence our first task is to determine possible Z decompositions or Z reductions for reducible Bravais arithmetic classes or, equivalently, for Bravais types of translation groups.

3.1. The plane groups

The oblique and rectangular systems are reducible. The first system admits an infinite set of inclined reductions; the second admits a unique orthogonal reduction, which results either in Z decomposition (primitive Bravais type p) or in Z reduction (centered Bravais type c).

The case of the oblique system illustrates the main problem of inclined reductions. Every basis $\{a, b\}$ of the oblique translation group implies Z decomposition $T(\mathbf{a}, \mathbf{b}) = T(\mathbf{a}) \oplus T(\mathbf{b})$. If we consider a Q reduction of V(T, Q), in which the G-invariant onedimensional subspaces of the space V(T, O) intersect with $T(\mathbf{a}, \mathbf{b})$ in the groups $T(\mathbf{a}')$, $T(\mathbf{b}')$ such that $\{\mathbf{a}', \mathbf{b}'\}$ is not a basis of $T(\mathbf{a}, \mathbf{b})$, we get, however, Z reduction of $T(\mathbf{a}, \mathbf{b})$ to the form of a subdirect sum $T(\mathbf{a}') \oplus T(b')[\mathbf{0} \cup \mathbf{d}_2 \cup \ldots \cup \mathbf{d}_n]$. Nevertheless, to each $T(\mathbf{a}')$ we can always find complementary $T(\mathbf{b}')$ such that $\{\mathbf{a}', \mathbf{b}'\}$ will be just another basis of $T(\mathbf{a}, \mathbf{b})$. Furthermore, there exists R reductions of V(T, R)that do not imply Q reductions. These are the cases when subspaces $V_1(R)$, $V_2(R)$ do not define 'crystallographic directions'. However, we can always find a translation group T for which a given R reduction implies Z decomposition. It is sufficient to take one vector of the basis of T in $V_1(k, R)$, the other in $V_2(h, R)$. We do not list such cases in the tables.

There are two Bravais types in the rectangular system. The primitive type leads to Z decomposition $T_p = T(\mathbf{a}, \mathbf{b}) = T(\mathbf{a}) \oplus T(\mathbf{b})$, the centered type to Z reduction $T_c = T(\mathbf{a}, \mathbf{b})[\mathbf{0} \cup (\mathbf{a} + \mathbf{b})/2] = T(\mathbf{a}) \oplus T(\mathbf{b})$ $[\mathbf{0} \cup (\mathbf{a} + \mathbf{b})/2]$ with G-invariant subgroups $T_{G1} =$ $T(\mathbf{a}), T_{G2} = T(\mathbf{b})$ and G-invariant projections $T_{G1}^0 =$ $T(\mathbf{a}/2), T_{G2}^0 = T(\mathbf{b}/2)$ of the group T_G . These simple results are collected in Table 1.

3.2. The space groups

All Z decompositions and Z reductions of the translation groups of the 11 reducible Bravais types are given in Table 2. The three-dimensional space can be reduced into two components only in such a way that one of the components is one dimensional, the second two-dimensional.

Convention. With the anticipation of further factorization and distribution of reducible space groups

Table 1. Reductions and decompositions of two-dimensional translation groups according to theirBravais classes

$$p = T(\mathbf{a}, \mathbf{b}); \ c = T[(\mathbf{a} + \mathbf{b})/2, (\mathbf{a} - \mathbf{b})/2];$$

$$\mu_a = T(\mathbf{a}); \ \mu_b = T(\mathbf{b}); \ \mu_{a/2} = T(\mathbf{a}/2); \ \mu_{b/2} = T(\mathbf{b}/2).$$

Oblique system			
Any basis vectors a , b	$T(\mathbf{a}) \oplus T(\mathbf{b})$	T ⁰ _{G1}	Т _{G2}
<i>P</i> :		∦a	∦ь
Rectangular system			
All reductions orthogonal	$T(\mathbf{a}, \mathbf{b}) \oplus T(\mathbf{c})$ $T(\mathbf{a}) \oplus T(\mathbf{b}) [0 \cup (\mathbf{a} + \mathbf{b})/2]$	T ⁰ _{G1}	Т _{G2}
p:		#a	#ь
c:		#a/2	#ь/2

into layer and rod classes, the following convention will be used throughout. The plane of the layer group will always be taken as the plane $V(\mathbf{a}, \mathbf{b})$, the axis of rod group as $V(\mathbf{c})$, where **a**, **b**, **c** are the vectors of the conventional unit cell. The symbol $T(\mathbf{a}, \mathbf{b})$ means the translation group generated by vectors **a**, **b**; the symbol $T(\mathbf{c})$ means the translation group generated by a single vector c. For each Bravais type of the translation subgroup T we give first its Z decomposition or Z reduction in the form of a direct or subdirect sum. respectively. In the right-hand column of Table 2 the groups $T_{G_1}^0$, $T_{G_2}^0$ are given, where index 1 corresponds to the projection σ_1 of the group T onto the plane $V(\mathbf{a}, \mathbf{b})$ and index 2 corresponds to the projection σ_2 onto the axis $V(\mathbf{c})$. The latter groups are given by lower-case letters p, c, which denote primitive or centered cases in the plane, and by h, which denotes one-dimensional translation groups. Further symbols used are explained in the table. The different crystallographic systems are commented on below.

Triclinic system. Each of the infinite number of possible choices of basis vectors **a**, **b**, **c** leads to a Z decomposition of the translation group T into a direct sum of $T(\mathbf{a}, \mathbf{b})$ and $T(\mathbf{c})$. We do not consider the Q and R reductions, which may lead to Z reduction or R reductions and which do not imply Q and Z reduction.

Monoclinic system. The system admits one orthogonal reduction and infinitely many inclined ones. There are two Bravais types - primitive and centered. According to our convention, we have to choose the unique axis along c for the orthogonal reduction. Then we get a Z decomposition for the first case and Z reduction in the second case, in three different forms according to the three cell choices in IT87. In cases of inclined reductions, the plane must necessarily contain the unique axis. The cases when the unique axis is either **a** or **b** are given. The vector c is assumed to complete the basis of primitive cases and to complete the conventional basis in centered cases. The latter admit Z decomposition for the choice of centering vector in the plane $V(\mathbf{a}, \mathbf{b})$: C centering; in this case, the centering vector completes the basis in the plane $V(\mathbf{a}, \mathbf{b})$ and c completes it to

Table 2. Reductions and decompositions of three-
dimensional translation groups according to their
Bravais classes

$$p = T(\mathbf{a}, \mathbf{b}), \ p_{\mathbf{a}/2} = T(\mathbf{a}/2, \mathbf{b}), \ p_{\mathbf{b}/2} = T(\mathbf{a}, \mathbf{b}/2), p_{\mathbf{a}/2, \mathbf{b}/2} = T(\mathbf{a}/2, \mathbf{b}/2), \ \hat{p} = T[(\mathbf{a}+\mathbf{b})/2, (\mathbf{a}-\mathbf{b})/2], c = T(\mathbf{a}) \oplus T(\mathbf{b})[\mathbf{0} \cup (\mathbf{a}+\mathbf{b})/2], \ \hat{p}_{1/3} = T[(2\mathbf{a}+\mathbf{b})/3, (\mathbf{a}+2\mathbf{b})/3], \not p = T(\mathbf{c}), \ \not p_{\mathbf{c}/2} = T(\mathbf{c}/2), \ \not p_{\mathbf{c}/3} = T(\mathbf{c}/3).$$

Triclinic system

Any basis vectors a , b , c	T_{G1}^0	T_{G2}^0
$P: T(\mathbf{a}, \mathbf{b}) \oplus T(\mathbf{c})$	p	ķ
Monoclinic systems		
Orthogonal reduction, unique axis c	T_{G1}^{0}	T_{G2}^0
$P: T(\mathbf{a}, \mathbf{b}) \oplus T(\mathbf{c})$	p	þ
A: $T(\mathbf{a}, \mathbf{b}) \oplus T(\mathbf{c})[0 \cup (\mathbf{b} + \mathbf{c})/2]$	Pb/2	#c/2
B: $T(\mathbf{a}, \mathbf{b}) \oplus T(\mathbf{c})[0 \cup (\mathbf{a} + \mathbf{c})/2]$	$p_{a/2}$	#c/2
I: $T(\mathbf{a}, \mathbf{b}) \oplus T(\mathbf{c})[0 \cup (\mathbf{a} + \mathbf{b} + \mathbf{c})/2]$	p	#c/2
Inclined reduction, unique axis a	T_{G1}^0	$T_{G_2}^0$
$P: T(\mathbf{a}, \mathbf{b}) \oplus T(\mathbf{c})$	p	þ
C: $T[(a+b)/2, (a-b)/2] \oplus T(c)$	с	þ
B: $T(\mathbf{a}, \mathbf{b}) \oplus T(\mathbf{c})[0 \cup (\mathbf{a} + \mathbf{c})/2]$	$p_{a/2}$	#c12
I: $T(\mathbf{a}, \mathbf{b}) \oplus T(\mathbf{c})[0 \cup (\mathbf{a} + \mathbf{b} + \mathbf{c})/2]$	с, -	ka12
Inclined reduction, unique axis b	T_{G1}^{0}	T_{G2}^{0}
$P: \qquad T(\mathbf{a}, \mathbf{b}) \oplus T(\mathbf{c})$	р.	h.
C: $T[(\mathbf{a}+\mathbf{b})/2, (\mathbf{a}-\mathbf{b})/2] \oplus T(\mathbf{c})$	c	ķ
A: $T(\mathbf{a}, \mathbf{b}) \oplus T(\mathbf{c})[0 \cup (\mathbf{b} + \mathbf{c})/2]$	Ph/2	Ha 12
I: $T(\mathbf{a}, \mathbf{b}) \oplus T(\mathbf{c})[0 \cup (\mathbf{a}+\mathbf{b}+\mathbf{c})/2]$	c	#c/2
Orthorhombic system		
All reductions orthogonal	T^0_{-}	T^0
P : $T(a, b) \oplus T(c)$	4 G1	* G2
$T[(a+b)/2] \oplus T(c)$	r c	<i>r</i>
$\begin{array}{ccc} \mathbf{B}: & T(\mathbf{a} \ \mathbf{b}) \oplus T(\mathbf{c}) \begin{bmatrix} 0 \ \mathbf{y} & \mathbf{c} \end{bmatrix} \oplus T(\mathbf{c}) \\ \mathbf{B}: & T(\mathbf{a} \ \mathbf{b}) \oplus T(\mathbf{c}) \begin{bmatrix} 0 \ \mathbf{y} & \mathbf{c} \end{bmatrix} \\ \end{array}$	n.	<i>#</i>
A: $T(a, b) \oplus T(c)[0 \cup (a + c)/2]$	Pa/2	#c/2
$F: T[(a+b)/2] \oplus T(c)[0 \cup (a+c)/2]$	P6/2	#c/2
$I: T(a, b) \oplus T(c)[0 \cup (a+b+c)/2]$	Pa/2,b/2 C	Fc/2
Tetragonal system		, _
	~ 0	0
All reductions orthogonal	T_{G1}	T_{G2}
$P: \qquad T(\mathbf{a}, \mathbf{b}) \oplus T(\mathbf{c})$	р	p
$T: T(\mathbf{a}, \mathbf{b}) \oplus T(\mathbf{c})[0 \cup (\mathbf{a} + \mathbf{b} + \mathbf{c})/2]$	p	# c/2
Hexagonal family		
All reductions orthogonal	T_{G1}^0	T_{G2}^0
Single Z decomposition (P) only in hexagonal system, both Z decomposition (P) and Z reduction (R) in trigonal system		
$P: T(\mathbf{a}, \mathbf{b}) \oplus T(\mathbf{c})$	р	k
R ₁ : (Obverse setting)	-	•
$T(\mathbf{a}, \mathbf{b}) \oplus T(\mathbf{c})[0 \cup (2\mathbf{a} + \mathbf{b} + \mathbf{c})/3$		
\cup (a +2 b +2 c)/3]	$\hat{p}_{1/3}$	He12
R_2 : (Reverse setting)	11/5	1.673
$T(\mathbf{a}, \mathbf{b}) \oplus T(\mathbf{c})[0 \cup (\mathbf{a} + 2\mathbf{b} + \mathbf{c})/3$		
$\cup (2\mathbf{a} + \mathbf{b} + 2\mathbf{c})/3]$	$\hat{p}_{1/3}$	10/2

the full basis. The other two choices of the unit cell lead to Z reductions.

Orthorhombic system. All three possible orthogonal reductions lead to Z decomposition for the primitive Bravais type. For the base-centered Bravais type, we get Z decomposition if the setting corresponds to C centering and Z reduction if the setting corresponds to A or B centering (as a consequence of our convention). Face- and volume-centered cases lead to Z reduction in all settings.

Tetragonal system. The unique orthogonal reduction leads to Z decomposition for the primitive Bravais type and to Z reduction for the *I*-centered Bravais type.

Hexagonal family. The unique orthogonal reduction leads to Z decomposition for the primitive Bravais type (in both hexagonal and trigonal systems) and to Z reduction for the rhombohedral Bravais type (trigonal system only). Both obverse and reverse settings are described. The groups T_{G1}^0 , T_{G2}^0 coincide for the two cases, as do the groups T_{G1}^0 , T_{G2}^0 ; the subdirect sums do not. This is due to different coupling of the coset representatives in the resolution of T_{G1}^0 , T_{G2}^0 versus T_{G1} , T_{G2} . The factor group $T_{G1}^0/T_{G1} \approx T_{G2}^0/T_{G2}$ is isomorphic to the cyclic group C_3 and the two different subdirect products are related to two automorphisms of C_3 (Kopský, 1988a). The resulting translation subgroups are distinct but each of them may be obtained from the other by a rotation on $\pi/3$ around the c axis.

4. An algebraic contra-practical factorization

Two methods of performing the factorization will be discussed briefly: an algebraic method and a method to determine factor groups directly from space-group diagrams, which is more practical and undoubtedly more appealing for crystallographers. In both cases, we assume that we are dealing with three-dimensional space groups. The procedure for plane groups is analogous.

An algebraic factorization

According to our convention, we consider space groups $\mathbb{G} = \{G, T_G, P, \mathbf{u}_G(g)\}$ in settings in which the subspaces $V(\mathbf{a}, \mathbf{b})$ and $V(\mathbf{c})$ are G-invariant. In this paper, only Z decompositions are considered so that T_G is a direct sum of translation subgroups in the two subspaces. As seen in Table 2, this means $T_G =$ $T_{G_1} \oplus T_{G_2} = T(\mathbf{a}, \mathbf{b}) \oplus T(\mathbf{c})$ for the primitive type or $T_G = T_{G_1} \oplus T_{G_2} = T[(\mathbf{a} + \mathbf{b})/2, (\mathbf{a} - \mathbf{b})/2] \oplus T(\mathbf{c})$ for the C setting of monoclinic and orthorhombic groups. According to the factorization procedure, the effect of homomorphisms σ_1 , σ_2 is to map the space group $\mathbb{G} = \{G, T_G, P, \mathbf{u}_G(g)\}$ respectively onto a contracted layer group $\mathbb{L} = \boldsymbol{\sigma}_1(\mathbb{G}) = [G, T_{G_1}, P_1, \mathbf{u}_{G_1}(g)]$ and onto a contracted rod group $\mathbb{R} = \sigma_2(\mathbb{G}) =$ $\langle G, T_{G2}, P_2, \mathbf{u}_{G2}(g) \rangle$, where $T_{G1}, \mathbf{u}_{G1}(g)$ and T_{G2} , $\mathbf{u}_{G2}(g)$ are projections of T_G , $\mathbf{u}_G(g)$ into subspaces $V_1(k, R)$ and $V_2(h, R)$.

The contracted layer groups, acting on $E(\mathbf{a}, \mathbf{b}) \times V(\mathbf{c})$, can be interpreted as Holser's 'groups of a two-sided plane', while the ordinary layer groups in $E(\mathbf{a}, \mathbf{b}, \mathbf{c})$ are Holser's 'sectional layer groups' (Holser, 1958). The algebraic determination of factor groups as contracted layer and rod groups is very simple. Their translation subgroups are already determined in Table 2. In the case of Z decompositions,

they coincide with groups T_{G1} , T_{G2} . The groups themselves are defined by components of the systems of nonprimitive translations in the two subspaces.

Factorization with use of space-group diagrams

In the preparation of the tables, the geometrical counterpart of the algebraic procedure was used. To perform the factorization in this way, we must understand its meaning and the meaning of components $\mathbf{u}_{G1}(g)$ and $\mathbf{u}_{G2}(g)$ of the system of nonprimitive translations in terms of graphical representations. We shall describe the procedure only for cases of orthogonal reductions and for space groups.

Layer classes

According to our convention, the factorization by the homomorphism σ_{ab} , which maps the space group onto the layer group, is always in the plane of the diagram, thus we have to neglect the components of nonprimitive translations along the c axis. Vol. A of International Tables for Crystallography (1987) contains diagrams that define all layer groups by projections σ_{ab} ; previous volumes do not. The addition of nonprimitive translations along the c axis changes the ordinary rotation axes to screw axes or adds a glide translation c/2 to planes that are perpendicular to the plane of the diagram. Axes and planes parallel with the plane of the diagram, inversion centers or rotoinversions are accordingly shifted along the c axis above the plane of the diagram. Hence, if we neglect the components of nonprimitive translations along the c axis, we convert space-group diagrams into layer-group diagrams by replacing all screw axes perpendicular to the diagram plane by ordinary ones, the dotted reflection planes (c/2) by full ones (0) and the dash-dotted planes $[(\mathbf{a}+\mathbf{b}+\mathbf{c})/2, (\mathbf{a}+\mathbf{c})/2 \text{ or}]$ $(\mathbf{b}+\mathbf{c})/2$] by dashed ones $[(\mathbf{a}+\mathbf{b})/2, \mathbf{a}/2 \text{ or } \mathbf{b}/2]$. Furthermore, we omit all fractions that indicate the location of parallel axes and planes, inversion centers and rotoinversions above the plane of the diagram.

Rod classes

To obtain the rod classes, we have to neglect components of the system of nonprimitive translations in the plane $V(\mathbf{a}, \mathbf{b})$ of the diagram, which vanish under the action of homomorphism $\boldsymbol{\sigma}_c$. The axis of the resulting rod group is perpendicular to the diagram in cases of orthogonal reductions and inclined otherwise (triclinic and monoclinic groups only). We may locate it at the upper left corner of the diagram and take it to be the origin. Ordinary and screw axes are related to this origin as well as planes that are perpendicular to the diagram; we have to replace the dashed plane symbols by solid lines and the dash-dotted by dotted lines while full and dotted lines remain unchanged, except for the shift towards the origin. Glide planes and twofold screw axes that are parallel to the diagram should be replaced by ordinary ones; the latter axes, inversion and rotoinversion centers should be shifted to pass through or be located at the origin and their heights above the diagram plane must be retained.

5. Hermann-Mauguin symbols for layer and rod groups

Whichever of the two methods we use to determine layer and rod groups as factor groups of reducible space groups, we face the same problem. Although the layer, rod and frieze groups have been known since 1929 – a rich year for groups that are now called subperiodic - neither generally accepted nor suitable standards and symbols have been available up to now. There is a plethora of notations starting from original papers (Alexander, 1929; Alexander & Hermann, 1928, 1929; Heesch, 1929; Hermann 1928, 1929; Weber, 1929) to tables of layer groups by Wood (1964) in the format of International Tables for Crystallography (1987), but none of them suits our purpose as well as the system now introduced, which is very close to the nomenclature of Bohm & Dornberger-Schiff (1967) and to recent tables by Grell, Krause & Grell (1989).

The principle of our notation is based on the existence of symmorphic representatives of layer and rod classes. To each contracted layer group $\mathbb{L} = [G, T(\mathbf{a}, \mathbf{b}), P_1, \mathbf{u}_{G1}(g)]$ we assign the symmorphic representative $\mathbb{G}_L = \{G, T(\mathbf{a}, \mathbf{b}, \mathbf{c}), P, \mathbf{u}_{G1}(g)\}$ of the layer class. We use exactly the same Hermann-Mauguin symbol for the layer group \mathbb{L} as for the group \mathbb{G}_L , except that the letter P is replaced by lower-case p or C is replaced by c. Analogously, to each contracted rod group $\mathbb{R} = \langle G, T(\mathbf{c}), P_2, \mathbf{u}_{G2}(g) \rangle$ there corresponds the symmorphic representative of the rod class, the space group $\mathbb{G}_R = \{G, T(\mathbf{a}, \mathbf{b}, \mathbf{c}), P, \mathbf{u}_{G2}(g)\}$, and we use its Hermann-Mauguin symbol for the rod group \mathbb{R} , replacing P by p.

Notice that in this way we shall obtain the symbols for all layer- and rod-group types including different settings and these will be correlated in the most natural way with symbols of reducible space-group types. A complete scheme calls, however, for correlation of origin choices, which needs separate consideration.

The origin of the long-known relationship between diagrams of layer groups and of certain space groups (Cochran, 1952), mentioned in the *Introduction*, now becomes clear. The diagram of every layer group \mathbb{L} can be interpreted as a diagram of the symmorphic representative \mathbb{G}_L of the layer class \mathbb{L} of space groups. An analogous and probably previously unnoted relationship exists between rod groups and certain space groups. The diagram of the symmorphic representative \mathbb{G}_R of a rod class \mathbb{R} contains some point such that its surrounding, containing symmetry elements that are either located at this point or pass through it, can be considered as a diagram of the corresponding rod group \mathbb{R} .

The two rectangular schemes for space groups of arithmetic classes 422P and 4mmP below illustrate the scheme and also the intersection theorem (paper *B*, theorem 2). The columns are headed by rod groups that identify the rod class to which the space groups of the column belong and rows are headed by symbols of layer groups that identify the layer classes to which the space groups of the row belong.

D_4	p422	\$4122	p4222	p4322
p422	P422	P4122	P4 ₂ 22	P4322
p4212	F 4212	F_{1212}	F 42212	647mc
040 p4mm	P4mm	P42cm	P4cc	P42mc
p4bm	P4bm	P42nm	P4nc	P42bc

The space groups in the first columns are the representative space groups of layer classes; the space groups in the first rows are the representatives of rod classes. Accordingly, they define the symbols of layer groups in the heading column and row. Each space group of the arithmetic class lies on the intersection of a layer and a rod class. The Hermann-Mauguin symbols are so ingeniously devised that we can trace in these schemes the rules by which the symbols of groups on intersections combine from symbols of symmorphic representatives. If we assign appropriate origins to layer, rod and space groups, then the shifts of origins of layer and rod groups will be reflected in such schemes as components of the shift of the space group on the intersection. Unfortunately, the origin choices of space-group diagrams in International Tables for Crystallography (1987) are not always compatible with this scheme.

6. Frieze classes of reducible plane groups with respect to Z decompositions

Plane and frieze groups act on Euclidean plane $E(\mathbf{a}, \mathbf{b})$. The contracted frieze groups act on a twosided line in a plane. Factor groups of reducible plane groups by partial-translation subgroups $T(\mathbf{a})$ or $T(\mathbf{b})$ then act on $V(\mathbf{a}) \times E(\mathbf{b})$ or $E(\mathbf{a}) \times V(\mathbf{b})$, respectively. As in the case of space groups we adopt the convention of always expressing the factorization with respect to the line $E(\mathbf{a}) \times V(\mathbf{b})$. The symbols of frieze groups are then identical with symbols of plane groups that are their symmorphic representatives, with p replaced by \not{e} . The three places in the symbols of frieze groups correspond subsequently to the direction perpendicular to the plane, to the direction of its translation subgroup and to the complementary direction in the plane. Accordingly, we get seven

 Table 3. Factorization of reducible plane groups with respect to Z decompositions

Its projections onto $V(\mathbf{a})$, $V(\mathbf{b})$			
σ_a	σ_b		
#1	<i>µ</i> 1		
# 2	# 2		
#1m1	#11m		
µ11m	µ1m1		
#1m1	#11g		
#11g	#1m1		
#2mm	#2mm		
#2mg	µ2mm		
#2mm	#2mg		
p2mg	∳2mg		
	Its projections onto σ_a #1 #2 #1m1 #1m #1m1 #1m #1m1 #1n1 #2mm #2mg #2mm #2mg		

Table 4. Distribution of reducible plane groups intofrieze classes with respect to Z decompositions

Frieze class	Plane groups
<i>p</i> 1	<i>p</i> 1
p2	p2
h11m	p11m(ab), p1g1(ab)
<i>k</i> 1 <i>m</i> 1	p1m1(ba)
∳11g	p11g(ba)
¢2mm	p2mm(ab, ba), p2gm(ba)
#2mg	p2mg(ab), p2gg(ab, ba)

symbols for frieze-group types: $\not = 1, \not = 2, \not = 1m1, \not = 11m$, $\not = 11g, \not = 2mm$ and $\not = 2mg$. Table 3 shows frieze groups as homomorphic images of plane groups with Zdecomposable translation subgroups. Pairs of plane groups connected by braces correspond to two settings, of which (*ab*) is the first, (*ba*) the second. The distribution of plane groups into frieze classes with respect to Z decompositions is given in Table 4.

7. Layer and rod classes of reducible space groups with respect to Z decompositions

In this section, we assign to each layer and rod class those reducible space groups that belong to it with respect to a particular Z decomposition. The general format of all tables is the same. In the first row we list the geometric classes by their Schönflies symbols and, next to this, the symbol of the arithmetic class. Apart from C settings of monoclinic and orthorhombic systems, all Bravais types are primitive. In the two columns we list the space groups of the layer and rod classes. The latter are denoted by Hermann-Mauguin symbols according to rules set in §5: for space groups, abbreviated Schönflies symbols are used which facilitate rapid searches in International Tables for Crystallography (1987). Only in the case of monoclinic groups are Hermann-Mauguin symbols also used to distinguish the setting and the cell choice. The first space group listed in each layer and rod class is its symmorphic representative and is printed in bold. If a rod class splits into two arithmetic rod classes then each has its own symmorphic representative. Underlined symmorphic representatives correspond to cases when the point group acts trivially on the subspace containing the translation subgroup by which we factorize. In these cases, the semidirectproduct form of the symmorphic representative turns into a direct product of the layer or rod group and of the translation subgroup of missing translations.

The layer groups are connected with plane groups as well as with space groups. The systems are named as a combination of the two characteristics: triclinic-oblique, monoclinic-oblique, monoclinicrectangular, orthorhombic-rectangular, tetragonalsquare, trigonal-hexagonal and hexagonal-hexagonal. In some cases, one part of the name implies the other. Monoclinic-inclined and monoclinicorthogonal rod groups should be distinguished. Triclinic rod groups are automatically inclined, all others are orthogonal.

7.1. Triclinic and monoclinic systems

These are the only two systems in which inclined reductions occur. Z decompositions of triclinic groups correspond to any choice of basis vectors a. b, c in the role of conventional vectors. The monoclinic system presents a special problem. From the viewpoint of reduction and factorization, the second edition of International Tables for Crystallography (1987) provides all necessary diagrams with the exception of a few in the monoclinic system. For Zdecompositions, these are the diagrams that would correspond to the Hermann-Mauguin symbols P1n1 or Pn11, P12/n1 or P2/n11 and P121/n11 or P21/n11. Both orthogonal and inclined reductions occur. The orthogonal reduction leads to an oblique system of layer groups and to an orthogonal system of rod groups. It is unique and, according to our convention, corresponds to the choice of the c axis as the unique monoclinic axis. This choice defines uniquely the conventional vector c but there are still infinitely many choices of conventional vectors a and **b**; space groups P112, P11m and P112/m have the same symbols whatever the choice of **a** and **b**. With every choice of **a**, **b** there are associated two other cell choices with respect to which the remaining three groups of the primitive Bravais type acquire three alternative symbols: (P11a, P11n, P11b), (P112/a, P112/n, P112/b) and $(P112_1/a, P112_1/n, P112_1/b)$, depending on the direction of the glide translation with respect to the conventional vectors **a** and **b**. Corresponding symbols p11a, p11n, p11b and p112/a, p112/n, p112/b denote two-layer group types with reference to three possible unit-cell choices in the plane (a, b).

Inclined reductions lead to rectangular systems for layer groups and to inclined systems for rod groups. The corresponding diagrams of monoclinic space

groups (on the right and below the oblique diagram) in IT87 are interpreted as orthogonal projections. The diagrams themselves do not depend on the choice of unique axis; the difference is in the labeling of axes. We adopt, in agreement with our convention, the position that the lower left and upper right diagrams correspond to the choice of c axis out of the plane of the diagram, while the edges of the rectangles are interpreted as the conventional vectors a and b. In addition, we consider the diagrams as skew projections of the groups in the direction of the c axis. The rules for geometrical factorization are the same as for orthogonal projections. The dotted line represents the glide plane and the nonprimitive translation c/2 is regarded as inclined to the diagram of the plane. Analogously, the fractions, which denote the heights above the diagram, now denote the shift in the direction inclined to the plane. The rod groups accordingly have c axes inclined to the plane of the diagram. The results of the factorization and classification of triclinic and monoclinic space groups are collected in Table 5.

7.2. Orthorhombic system

Each orthorhombic group can be and in IT87 actually is presented in six settings, which correspond to three possible orthogonal reductions. We interpret the diagrams according to our convention in such a way that the c axis is always perpendicular to the plane of the diagram; the edges of rectangles are assumed to correspond to vectors a and b, where a corresponds to the vertical, **b** to the horizontal edge. If we rotate the page by 90°, the vectors **a** and **b** interchange. Thus, instead of considering three reductions of a given group, we consider one reduction of the six possible settings. Accordingly, the layer groups appear generally in two possible settings that sometimes lead to the same symbol. In Table 6, for each layer and rod group, the Schönflies symbols of all space groups for which they are the factor group are given, with the settings in which factorization by $T(\mathbf{c})$ and $T(\mathbf{a}, \mathbf{b})$ will provide these groups given in parentheses.

7.3. Tetragonal system

Since the groups of this system admit just one orthogonal reduction, there are no specific problems connected with their factorization. Note, however, the already-mentioned fact that in Table 7 there are pairs of rod groups where the two rod groups of the same type define different space-group types as a result of their different orientation with respect to the translation subgroup $T(\mathbf{a}, \mathbf{b})$. The rod groups of the same type are linked by braces in Table 7, which presents layer and rod classes of tetragonal space groups.

Geometric- arithmetic class		Layer classes		Rod classes
Triclinic system		Oblique system		Inclined
$C_1 - 1P$	<i>p</i> 1	C_1^1	<i>#</i> 1	C_1
$C_i - \overline{1}P$	pī	$\overline{C_i^1}$	# Ī	$\overline{C_{i}^{1}}$
Monoclinic system		Oblique system		Orthogonal
Orthogonal reduction				
C ₂ -112P	p112	$\underline{C_2^1}, C_2^2$	#112 #112	C_2^1 C_2^2
C_s-11mP	p11m	C ¹ _s	µ11m	C_s^1, C_s^2
	p11a			
	p11n } p11b }	C_s^2		
C_{2h} -112/mP	p112/m	C_{2h}^{1}, C_{2h}^{2}		
	p112/a			
	p112/n	C_{2h}^{4}, C_{2h}^{5}	$\mu 112_1/m$	C_{2h}^2, C_{2h}^5
	p112/b]			
Monoclinic system		Rectangular system		Inclined
Inclined reduction, unique	e axis b			
C ₂ -121 <i>P</i>	p121	$C_{2}^{1}(P121)$	¢121	$C_2^1(p121), C_2^2(P12_11);$
	<i>p</i> 12 ₁ 1	$C_2^2(P12_11)$		$C_2^3(C121)$
-121 <i>C</i>	c121	$C_{2}^{2}(C121)$		
$C_{s}-1m1P$	p1m1	$\underline{C_s^1}(\underline{P1m1}), C_s^2(P1c1)$	#1m1	$C_{s}^{1}(P1m1), C_{s}^{2}(P1a1);$
	p1a1	$\frac{C_s^2}{(P1a1, P1n1)}$		$C_s^3(C1m1)$
-1m1C	c1m1	$\underline{C_s^3}(\underline{C1m1}), C_s^4(C1c1)$	#1c1	$C_{s}^{2}(P1c1, P1n1);$
				$C_{s}^{4}(C1c1)$
$C_{2h} - 12/m1P$	p12/m1	C_{2h}^{1} (P12/m1), C_{2h}^{4} (P12/c1)	h^{12}/m^{12}	C_{2h}^{1} (P12/m1), C_{2h}^{2} (P12 ₁ /m1),
	$p12_{1}/m1$	$C_{2h}^{2}(P12_{1}/m1), C_{2h}^{5}(P12_{1}/c1)$		$C_{2h}^{4}(P12/a1), C_{2h}^{5}(P12_{1}/a1);$
	p12/a1	C_{2h}^4 (P12/a1, P12/n1)		$C_{2h}^{3}(C12/m1)$
	p12 ₁ /a1	$C_{2h}^{5}(P12_{1}/a1, P12_{1}/n1)$	#12/c1	C_{2h}^{4} (P12/c1, P12/n1), C_{2h}^{5} (P12 ₁ /c1, P12 ₁ /n1)
-12/m1C	c12/m1	$C_{2h}^{3}(C12/m1), C_{2h}^{6}(C12/c1)$		$C_{2h}^{6}(C12/c1)$
Inclined reduction, unique	e axis a			
C ₂ -211 <i>P</i>	p211	$C_{2}^{1}(P211)$	¢211	$C_2^1(P211), C_2^2(P2_111);$
	<i>p</i> 2 ₁ 11	$C_{2}^{2}(P2_{1}11)$		$C_2^3(C211)$
-211 <i>C</i>	c211	$C_{2}^{2}(C211)$		
$C_s - m 11P$	pm11	$\underline{C_s^1}(\underline{Pm11}), C_s^2(Pc11)$	<i>pm</i> 11	$C_{s}^{1}(Pm11), C_{s}^{2}(Pa11);$
	pb11	$\frac{C_s^2}{(Pb11, Pn11)}$		$C_{s}^{3}(Cm11)$
-m11C	<i>cm</i> 11	$\underline{C_s^3}(\underline{Cm11}), C_s^4(Cc11)$	<i>p</i> c11	$C_{s}^{2}(Pc11, Pn11);$
				C_s^4 (Cell)
$C_{2h}-2/m11P$	p2/m11	$C_{2h}^{1}(P2/m11), C_{2h}^{4}(P2/c11)$	#2/m11	$C_{2h}^{1}(P2/m11), C_{2h}^{2}(P2_{1}/m11),$
	$p2_1/m11$	$C_{2h}^{2}(P2_{1}/m11), C_{2h}^{5}(P2_{1}/c11)$		$C_{2h}^{4}(P2/b11), C_{2h}^{5}(P2_{1}/b11);$
	p2/b11	C_{2h}^{4} (P2/b11, P2/n11)		$C_{2h}^{3}(C2/m11)$
	$p2_{1}/b11$	$C_{2h}^{5}(P2_{1}/b11, P2_{1}/n11)$	\$2/c11	C_{2h}^{4} (P2/c11, P2/n11), C_{2h}^{5} (P2 ₁ /c11, P2 ₁ /n11);
-2/m11c	c2/m11	$C_{2h}^{3}(C2/m11), C_{2h}^{6}(C2/c11)$		$C_{2h}^{6}(C2/c11)$

Table 5. Layer and rod classes of reducible space groups with respect to Z decompositions of their translation subgroups: triclinic and monoclinic systems

Geometric- arithmetic class Orthorhombic system		Layer classes Rectangular system		Rod classes Orthogonal
ברר ה גרו ה	n777	$D^{1}(a l)$ $D^{2}(abc bac)$	#222	$D_1^1(all), D_2^2(acb, cab, cba, bca), D_2^3(acb, cab);$
$D_2 - 2221$	$(n^2, 2^2)$	$D_2^2(ab, ba)$, $D_2^3(acb, bca)$,	$D_2^6(abc, bac)$
	n22.2	$D_{2}^{2}(acb, bca), D_{3}^{2}(cab, cba)$	#222 ₁	$D_2^2(abc, bac), D_2^3(acb, cab, cba, bca), D_2^4(all);$
	p2,2,2	$D_{2}^{3}(abc, bac), D_{2}^{4}(all)$		$D_2^4(abc, bac)$
-222 <i>C</i>	c222	$D_2^{\tilde{6}}(abc, bac), D_2^{\tilde{5}}(abc, bac)$		
C _{2v} -mm2P	pmm2	$\underline{C_{2v}^1}(abc, bac), C_{2v}^2(abc, bac), C_{2v}^3(abc, bac)$	¢mm2	$C_{2v}^{1}(abc, bac), C_{2v}^{4}(abc, bac), C_{2v}^{8}(abc, bac);$ $C_{2v}^{1}(abc, bac)$
	pma2	$\underline{C_{2\nu}^{4}}(abc), C_{2\nu}^{5}(abc), C_{2\nu}^{6}(bac), C_{2\nu}^{7}(abc)$	$\int \mu mc2_1$	$C_{2v}^{2}(abc), C_{2v}^{5}(bac), C_{2v}^{7}(abc), C_{2v}^{9}(bac);$ $C_{2v}^{12}(abc)$
	pbm2	$\underline{C_{2v}^{4}}(bac), C_{2v}^{5}(bac), C_{2v}^{6}(abc), C_{2v}^{7}(bac)$	<i>µcm</i> 2 ₁	$C_{2v}^{2}(bac), C_{2v}^{5}(abc), C_{2v}^{7}(bac), C_{2v}^{9}(abc);$ $C_{2v}^{12}(bac)$
	pba2	$\underline{C_{2v}^8}(abc, bac), C_{2v}^9(abc, bac), C_{2v}^{10}(abc, bac)$	pcc2	$C_{2v}^{3}(abc, bac), C_{2v}^{6}(abc, bac), C_{2v}^{10}(abc, bac);$ $C_{2v}^{13}(abc, bac)$
-mm2C	cmm2	$C_{2v}^{11}(abc, bac), C_{2v}^{12}(abc, bac), C_{2v}^{13}(abc, bac)$		
$C_{2} - m^2 m P$	nm2m	$\overline{C_{2n}^1}(acb, bca), C_{2n}^4(bca)$	(<u>k</u> m2m	$C_{2\nu}^1(acb, bca), C_{2\nu}^2(acb, bca), C_{2\nu}^3(acb, bca),$
-2mmP	p^{2mm}	$C_{2\nu}^{1}(cab, cba), C_{2\nu}^{4}(cba)$]	$C_{2v}^{4}(acb), C_{2v}^{5}(acb), C_{2v}^{6}(bca), C_{2v}^{7}(acb);$
	$pm2_1b$	$C_{2p}^{2}(acb), C_{2p}^{5}(bca)$	1	$C_{2v}^{14}(bca), C_{2v}^{15}(bca)$
	$p2_1ma$	$C_{2\nu}^2(cab), C_{2\nu}^5(cba)$	(µm2m	$C_{2\nu}^1(cab, cba), C_{2\nu}^2(cab, cba), C_{2\nu}^3(cab, cba),$
	$pb2_1m$	$C_{2v}^2(bca), C_{2v}^7(bca)$		$C_{2\nu}^{4}(cab), C_{2\nu}^{5}(cab), C_{2\nu}^{6}(cba), C_{2\nu}^{\prime}(cab);$
	$p2_1am$	$C_{2v}^2(cba), C_{2v}^7(cba)$		$C_{2\nu}^{14}(cba), C_{2\nu}^{15}(cba)$
	∫pb2b	$C^3_{2v}(acb, bca), C^6_{2v}(acb)$	(pc2m	$C_{2v}^{4}(bca), C_{2v}^{3}(bca), C_{2v}^{0}(acb), C_{2v}^{1}(bca),$
	(p2aa	$C^3_{2\nu}(cab, cba), C^6_{2\nu}(cab)$	Į	$C_{2\nu}^{\circ}(acb, bca), C_{2\nu}^{\circ}(acb, bca), C_{2\nu}^{\circ}(acb, bca);$
	{pm2a	$C_{2v}^4(acb), C_{2v}^8(acb, bca)$		$C_{2v}^{\circ}(bca), C_{2v}^{\circ}(bca)$
	p2mb	$C_{2\nu}^4(cab), C_{2\nu}^8(cab, cba)$	(#2cm	$C_{2v}(cba), C_{2v}(cba), C_{2v}(cab), C_{2v}(cba),$
	∫pb2₁a	$C_{2\nu}^{5}(acb), C_{2\nu}^{9}(acb)$		$C_{2\nu}^{\circ}(cab, cba), C_{2\nu}^{\circ}(cab, cba), C_{2\nu}^{\circ}(cab, cba);$
	$p_{1}ab$	$C_{2v}^{2}(cab), C_{2v}^{2}(cab)$		$C_{2\nu}(cba), C_{2\nu}(cba)$
] pb2n	$C_{2v}(bca), C_{2v}(acb, bca)$		
	(p2an	$C_{2\nu}^{2}(cba), C_{2\nu}^{2}(cab, cba)$		
	$pm 2_1 n$	$C_{2\nu}(acb), C_{2\nu}(bca)$		
	(p_{2},mn)	$C_{2v}(cab), C_{2v}(cba)$		
-m2mc	<i>cm2m</i>	$C_{2v}(bca), C_{2v}(bca)$		
-2 <i>mm</i> C	(am2a	$C_{20}^{15}((bca), C_{20}^{17}(bca))$		
	c2mb	$C_{20}^{15}(cba)$ $C_{20}^{17}(cba)$		
	(021110	$D_{20}^{1}(200), C_{20}^{2}(200)$	/. m . m . m .	\mathbf{D}^{1} (all) \mathbf{D}^{3} (ach call cha hea) \mathbf{D}^{4} (all heac)
D_{2h} -mmmP	pmmm	$D_{2h}^{3}(all), D_{2h}^{2}(abc, bac), D_{2h}^{2}(cba, bca)$	µ mmm	$D_{2h}^{s}(abc, bac, acb, cab)$, $D_{2h}^{r}(acb, cab)$, $D_{2h}^{r}(abc, bac)$
	pomo	$D_{2h}(acb, cba), D_{2h}(cab, cba), D_{2h}(bac), D_{2h}(bca)$ $D_{3}^{3}(acb, bcc), D_{4}^{4}(acb, cba), D_{7}^{7}(abc), D_{8}^{8}(cba)$		$D_{2h}^{8}(acb, cab) D_{2h}^{9}(abc, bac) D_{2h}^{11}(cba, bca),$
	(pmaa phan	$D_{2h}(cab, bca), D_{2h}(acb, cba), D_{2h}(abc), D_{2h}(cba)$		$D_{2h}^{13}(abc, bac); D_{2h}^{19}(abc, bac), D_{2h}^{21}(abc, bac)$
	(nmma	$D_{2h}^{5}(abc), D_{k}^{8}(abc), D_{2h}^{9}(abc), Cab)$	kccm	$D_{2h}^{3}(abc, bac), D_{2h}^{2}(all), D_{2h}^{4}(acb, cab, cba, bca),$
) pmmb	$D_{2h}^{5}(ac), D_{2h}^{8}(ac), D_{2h}^{9}(ac), b_{2h}^{1}(ac)$,	$D_{2h}^6(abc, bac, cba, bca), D_{2h}^7(cba, bca),$
	(pmam	$D_{2h}^{5}(acb), D_{2h}^{7}(cba), D_{2h}^{11}(bac), D_{2h}^{13}(acb, bca)$		$D_{2h}^{8}(abc, bac), D_{2h}^{10}(abc, bac), D_{2h}^{12}(abc, bac),$
	phinant phmm	$D_{2h}^{5}(cab), D_{2h}^{7}(bca), D_{2h}^{11}(abc), D_{2h}^{13}(cab, cba)$		$D_{2h}^{14}(abc, cab); D_{2h}^{20}(abc, bac), D_{2h}^{22}(abc, bac)$
	(poman	$D_{2h}^{7}(acb), D_{2h}^{6}(cba), D_{2h}^{12}(cab, cba), D_{2h}^{13}(bac)$	(pmcm	$D_{2h}^{5}(bca), D_{2h}^{6}(cab), D_{2h}^{7}(abc), D_{2h}^{8}(bca),$
	bmn	$D_{2h}^{7}(cab), D_{2h}^{6}(bca), D_{2h}^{12}(acb, bca), D_{2h}^{13}(abc)$		$D_{2h}^{9}(cab, cba), D_{2h}^{10}(acb, bca), D_{2h}^{11}(abc, cab),$
	(pbab	$D_{2h}^{8}(acb), D_{2h}^{6}(bac), D_{2h}^{10}(acb, bca), D_{2h}^{14}(cba)$		$D_{2h}^{12}(cab, cba), D_{2h}^{13}(acb, bca), D_{2h}^{14}(abc, bca),$
	pbaa	$D_{2h}^{8}(cab), D_{2h}^{6}(aca), D_{2h}^{10}(cab, cba), D_{2h}^{14}(bca)$	{	$D_{2h}^{15}(abc, cab, bca), D_{2h}^{16}(bac, cab, bca);$
				$D_{2h}^{17}(abc), D_{2h}^{18}(abc),$
	pbam	$D_{2h}^{9}(abc, bac), D_{2h}^{12}(abc, bac), D_{2h}^{16}(acb, cab)$	<i>µ</i> cmm	$D_{2h}^{2}(cba), D_{2h}^{o}(acb), D_{2h}'(bac), D_{2h}^{o}(cba),$
	f pmab	$D_{2h}^{11}(cba), D_{2h}^{14}(acb), D_{2h}^{15}(bac, acb, cba), D_{2h}^{16}(bac)$	l	$D_{2h}^{r}(acb, bca), D_{2h}^{r}(cab, cba), D_{2h}^{r}(bac, acb),$
	{ pbma	$D_{2h}^{11}(bca), D_{2h}^{14}(cab), D_{2h}^{15}(abc, cab, bca), D_{2h}^{16}(abc)$		$D_{2h}^{i}(acb, bca), D_{2h}^{i}(cab, cba), D_{2h}^{i}(bac, cba),$
	pmmn	$D_{2h}^{13}(abc, bac), D_{2h}^{10}(abc, bac), D_{2h}^{10}(cba, bca)$		$D_{2h}^{*}(bac, acb, cba), D_{2h}^{*}(abc, acb, cba);$
-mmmC	cmmm	$D_{2h}^{19}(abc, bac), D_{2h}^{10}(abc, bac), D_{2h}^{20}(abc, bac)$		$D_{2h}(bac), D_{2h}(bac)$
cm	ma = cmmb	$D_{2h}^{\prime}(abc, bac), D_{2h}^{\prime}(abc, bac), D_{2h}^{\prime}(abc, bac)$		

Table 6. Layer and rod classes of reducible space groups with respect to Z decompositions of their translation subgroups: orthorhombic system

arithmetic class	I	ayer classes	R	od classes
Tetragonal system	S	quare system	C	Orthogonal
C_4-4P	<i>p</i> 4	$C_{4}^{1}, C_{4}^{2}, C_{4}^{3}, C_{4}^{4}$	<i>k</i> 4	C ¹
			<i>k</i> 4,	C_4^2
			k47	C_{4}^{3}
			<i>#</i> 4 ₃	C_4^4
$S_4 - \bar{4}P$	p4	S_4^1	¢4	S4
C_{4h} -4/mP	p4/ m	C_{4h}^1, C_{4h}^2	<i>⊭</i> 4/ <i>m</i>	C^1_{4h}, C^3_{4h}
	p4/ n	C_{4h}^3, C_{4h}^4	$\mu 4_2/m$	C_{4h}^2, C_{4h}^4
D ₄ -422 <i>P</i>	p422	$D_4^1, D_4^3, D_4^5, D_4^7$	k422	D^1 , D^2
	p4212	$D_4^2, D_4^4, D_4^6, D_4^8$, ∳4₁22	D_4^3, D_4^4
			#4 ₂ 22	D_4^5, D_4^6
			# 4₃22	D_4^7, D_4^8
C_{4v} -4mmP	p4mm	$C_{4v}^1, C_{4v}^3, C_{4v}^5, C_{4v}^7$	∳4mm	C_{4n}^{1}, C_{4n}^{2}
	p4bm	$\overline{C_{4v}^2}, C_{4v}^4, C_{4v}^6, C_{4v}^8$	{ #4 ₂ cm	C_{4v}^{3}, C_{4v}^{4}
			{ #42mc	C_{4v}^7, C_{4v}^8
			#4cc	C_{4v}^5, C_{4v}^6
$D_{2d} - \bar{4}2mP$	p42m	D_{2d}^1, D_{2d}^2	(#42m	D_{2d}^{1}, D_{2d}^{3}
	p421m	D_{2d}^3, D_{2d}^4	{{#42c	D_{2d}^2, D_{2d}^4
- 4 m2P	pām2	D_{2d}^{5}, D_{2d}^{6}	{ [#ām2	D_{2d}^5, D_{2d}^7
	p4b2	D_{2d}^7, D_{2d}^8	<i>↓</i> 4c2	D_{2d}^{6}, D_{2d}^{8}
D_{4h} -4/mmmP	p4/mmm	$D^1_{4h}, D^2_{4h}, D^9_{4h}, D^{10}_{4h}$	#4/ mmm	$D_{4h}^1, D_{4h}^3, D_{4h}^5, D_{4h}^7$
	p4/nbm	$D_{4h}^3, D_{4h}^4, D_{4h}^{11}, D_{4h}^{12}$	#4/ mcc	$D_{4h}^2, D_{4h}^4, D_{4h}^6, D_{4h}^8$
	p4/mbm	$D_{4h}^5, D_{4h}^6, D_{4h}^{13}, D_{4h}^{14}$	#42/mmc	$D_{4h}^9, D_{4h}^{11}, D_{4h}^{13}, D_{4h}^{15}$
	p4/ nmm	$D_{4h}^7, D_{4h}^8, D_{4h}^{15}, D_{4h}^{16}$	#4 ₂ / mcm	$D_{4h}^{10}, D_{4h}^{12}, D_{4h}^{14}, D_{4h}^{16}$

Geometric-

 Table 7. Layer and rod classes of reducible space groups with respect to Z decompositions of their translation subgroups: tetragonal system

7.4. Hexagonal family.

This family splits into trigonal and hexagonal systems and the layer and rod classes are accordingly listed in Tables 8 and 9. Again, there are no specific problems connected with factorization. It is, perhaps, worth observing that each arithmetic rod class in this family consists of just one space-group type. This is a direct consequence of the fact that the plane hexagonal Bravais type relates exactly one layer group to each point group.

8. Enantiomorphism

The origin of enantiomorphism in three dimensions is characterized in §2 of paper B as the screw enantiomorphism. 10 of the 11 enantiomorphic pairs of space groups are reducible and their enantiomorphism is a consequence of the enantiomorphism of corresponding rod groups. Theoretically, enantiomorphism of a subperiodic group results in enantiomorphic class in question. We list all enantiomorphic pairs of space groups and of corresponding rod classes in Table 10. There are only two cases in which the enantiomorphic rod classes contain more than one (in particular two) enantiomorphic space-group types.

Table 8. Layer and rod classes of reducible space groups with respect to Z decompositions of their translation subgroups: hexagonal family/trigonal system

class	Layer classes			Rod classes		
Trigonal system	Hexag	onal system		Ortho	gonal	
C ₃ -3P	<i>p</i> 3	C_3^1, C_3^2, C_3^3	#3		C_2^1	
			#3 ₁		C_{3}^{2}	
			#3 ₂		C_{3}^{3}	
C_{3i} - $\overline{3}P$	p3	C_{3i}^{1}	#3		C_{3i}^{1}	
D ₃ -312P	p312	D_3^1, D_3^3, D_3^5	#312	D_{3}^{1}	#321	D_3^2
-321 <i>P</i>	p321	D_3^2, D_3^4, D_3^6	#3 ₁ 12	$D_{3}^{3};$	#3 ₁ 21	D_3^4
			#3 ₂ 12	$D_{3}^{5};$	#32.21	D_3^6
C _{3c} -3m1P	p3m1	C_{3v}^1, C_{3v}^3	#3m1	$C_{3v}^{1};$	#31m	C_{3v}^{2}
-31 <i>mP</i>	p31m	$\underline{C_{3v}^2}, C_{3v}^4$	#3c1	$C_{3v}^{3};$	#31c	C ⁴ _{3v}
D_{3d} - $\overline{3}12/mP$	p312/m	$D_{3d}^1, D_{3d}^2;$	#312/m	D_{3d}^1	#32/m1	
$-\bar{3}2/m1P$	p32/m1	D_{3d}^3, D_{3d}^4	#312/c	D_{3d}^2 ;	#32/c1	D_{3d}^4

9. Concluding remarks

The factorization of reducible space (plane) groups by partial-translation subgroups refines our knowl-

Geometric

Geometric- arithmetic class		Layer classes		Rod cla	isses	
Hexagonal system	ı H	exagonal system		Orthog	onal	
C ₆ -6P	<i>p</i> 6	$C_6^1, C_6^2, C_6^3, C_6^4, C_6^5, C_6^6$	#6	C_{6}^{1}	#6 ₂	C ₆ ⁴
		—	#6 ₁	C_6^2	#65	C_6^3
			#6 ₃	C 6	<i>p</i> 64	C 56
$C_{3h} - \bar{6}P$	рō	C_{3h}^{1}	ħĞ	C_{3}^{1}		
C _{6h} -6/mP	p6/ m	C_{6h}^{1}, C_{6h}^{2}	µ6/m	C_{6h}^1	µ6₃/m	C ² _{6h}
D ₆ -622 P	p622	$D_6^1, D_6^2, D_6^3, D_6^4, D_6^5, D_6^6$	<i>µ</i> 622	D_6^1	#6 ₃ 22	D_6^4
Ū			#6 ₁ 22	D_6^2	#6 ₅22	D_6^3
			#6 ₃ 22	D_{6}^{6}	#6 ₄ 22	D 6
$D_{3h}-\bar{6}m2P$	p ē m2	D_{3h}^{1}, D_{3h}^{2}	µ6m2	$D_{3h}^{1};$	#62m	D ³ _{3h}
- <u>6</u> 2mP	p ö 2m	D_{3h}^3, D_{3h}^4	#6c2	D_{3h}^2 ;	462c	D ⁴ _{3h}
C_{6v} -6mmP	p6mm	$C^{1}_{6v}, C^{2}_{6v}, C^{3}_{6v}, C^{4}_{6v}$	#6mm	C_{6v}^1	#6cc	C_{6v}^{2}
			463cm	$C_{6v}^{3};$	µ6₃mc	C ⁴ ₆₀
D _{6h} -6/mmmP	p6/mmm	$D^1_{6h}, D^2_{6h}, D^3_{6h}, D^4_{6h}$	46/ mmm	D_{6h}^{1}	46/mcc	D_{6k}^{2}
			µ6/ mcm	$D_{6h}^{3};$	#6/ mmc	D_{6h}^4

 Table 9. Layer and rod classes of reducible space groups with respect to Z decompositions of their translation

 subgroups: hexagonal family/hexagonal system

edge of their structure, perfects their systemization and, at least in our opinion, provides the most logical nomenclature for frieze, layer and rod groups. Further important consequences stem from representation theory. The homomorphisms σ_1 , σ_2 with kernels ker $\sigma_1 = T_{G2}$, ker $\sigma_2 = T_{G1}$ map the group G onto layer group $\mathbb{L} = \sigma_1(\mathbb{G})$ and rod group $\mathbb{R} = \sigma_2(\mathbb{G})$ in the same way that the homomorphism σ with kernel ker $\sigma = T_G$ maps it onto the point group $G = \sigma(\mathbb{G})$. The impact of this last relation is well known: firstly, the lattice of equitranslational subgroups of the group G is isomorphic to the lattice of subgroups of the point group G and, secondly, all representations of the group G, corresponding to the wave vector $\mathbf{k} = \mathbf{0}$, are engendered by representations of the point group G. The usefulness of these relationships is well known to phase-transition theorists. Ascher (1968) used the isomorphism of lattices to tabulate lattices of equitranslational subgroups of space groups. The use of analogous relations stemming from partial factorization in a joint systemization of representations and lattices of space and subperiodic groups is discussed by Kopský (1988b).

Finally, it is worth mentioning the existence of a problem that is important in the theory of interfaces in crystals such as domain walls (see, for example, Janovec, Schranz, Warhanek & Zikmund, 1989) or twin and grain boundaries. We refer to it as to the 'scanning of layer groups' (Kopský & Litvin, 1988; Janovec, Kopský & Litvin, 1988; Kopský, 1990) and formulate it as follows: given a space group and a direction of a plane $V(\mathbf{a}', \mathbf{b}', \mathbf{c}')$, find the symmetries of plane cuts of the crystal as the plane is shifted in space. As will be shown in other publications (Kopský, 1992), the classification of space groups

Table 10. Enantiomorphic pairs of space groups and corresponding enantiomorphic pairs of their rod classes

	Space			Space	
No.*	group	Rod	l class	group	No.*
IT 76	$C_{4}^{2}(P4_{1})$	<i>µ</i> 4 ₁	#4 ₃	$C_{4}^{4}(P4_{3})$	IT 78
IT 91	$D_4^3(P4_122)$	(4 . 2 2	(4.22	$\int D_4^7 (P4_322)$	IT 95
IT 92	$D_4^4(P4_12_12)\int$	µ4133	\$4322 ·	$D_4^8(P4_32_12)$	IT 96
IT 144	$C_{3}^{2}(P3_{1})$	#31	#32	$C_{3}^{3}(P3_{2})$	IT 145
IT 151	$D_{3}^{3}(P_{1}^{3}12)$	43.2	43-2	$\int D_3^5(P3_212)$	IT 153
IT 152	$D_{3}^{4}(P_{1}^{2}21)\int$	1.212	1022	$D_{3}^{6}(P3_{2}^{-}21)$	IT 154
IT 169	$C_6^2(P6_1)$	#6 ₁	#6 ₅	$C_6^3(P6_5)$	IT 170
<i>IT</i> 171	$C_{6}^{4}(P6_{2})$	#6 ₂	þ64	$C_{6}^{5}(P6_{4})$	IT 172
IT 178	$D_6^2(P6_122)$	#6 ₁ 22	¢6522	$D_6^4(P6_522)$	IT 179
<i>IT</i> 180	$D_6^4(P6_222)$	£6222	<i>µ</i> 6₄22	$D_6^5(P6_422)$	<i>IT</i> 181

* Number in International Tables for Crystallography (1983).

into layer and rod classes is the first step to the solution of this problem.

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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 Qreductions that lead to Z reduction but not to Zdecomposition. 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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