

# Unified system of Hermann–Mauguin symbols for groups of material physics. 1. Groups with decomposable lattices

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The system of Hermann–Mauguin symbols for space and subperiodic Euclidean groups in two and three dimensions is extended to groups with continuous and semicontinuous translation subgroups (lattices). An interpretation of these symbols is proposed in which each symbol defines a quite specific Euclidean group with reference to a crystallographic basis, including the location of the group in space. Symbols of subperiodic (layer and rod) groups are strongly correlated with symbols of decomposable space groups on the basis of the factorization theorem. Introduction of groups with continuous and semicontinuous lattices is connected with a proposal for several new terms that describe the properties of these groups and with a proposal to amend the meaning of space groups and of crystallographic groups. Charts of plane, layer and space groups describe variants of these groups with the same reducible point group but various types of lattices. Examples of such charts are given for plane, layer and space groups to illustrate the unification principle for groups with decomposable lattices.

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## 1. A brief history and the current status of symbols

Most mathematicians who specialize in some branch of group theory would be surprised to hear that groups are of specific importance in physics. Actually, group theory is even connected with such basic laws of nature as the conservation of momentum and of angular momentum. In classical physics, we believe that our space is of Euclidean character, so that it is homogeneous and isotropic. In group-theoretical language, it means that the space is invariant under translations and under rotations about any chosen point. Conservation of momentum is a consequence of this translational symmetry, conservation of angular momentum follows from the rotational symmetry. In the theory of special relativity, the law of the conservation of the energy-momentum tensor also follows from Minkowski's metric of space–time.

Groups are also a mathematical tool for the consideration of symmetry and its consequences in material physics. Point groups were originally introduced in connection with classification of the external shape of monocrystals into so-called Hessel–Gadolin classes. Later, Fedorov and Schoenflies derived independently the 230 types of possible space symmetries of crystals. Neither of these two authors completely succeeded on their first attempts, and finally they compared their results which were also confirmed by Barlow. It is remarkable that the basic assumption of this derivation,

namely the periodic structure of crystals, was convincingly experimentally confirmed only after the discovery of X-rays and of diffraction methods which came about two decades later.

The description and symbols for space groups are presented in Vol. A, *Space Group Symmetry* of the *International Tables for Crystallography* (1983) (abbreviated here as *ITA*). In this volume, one can find two kinds of symbols for the point and space groups: the Schoenflies and the Hermann–Mauguin symbols. Since the first edition of this book in 1930, crystallography has developed into a specific branch of physical science, the importance of which can be hardly overestimated. Technological applications of crystals are amongst the pillars of modern civilization, especially in communication technology and it is not an exaggeration if we claim that crystals helped to change our world positively in many aspects. The number of known crystal structures today is hundreds of thousands and it is therefore important that there exist generally approved and used standards for their description as given in *ITA*. The tables themselves, as well as the Hermann–Mauguin symbols, have consequently been developed to their present form. The last amendment concerned the introduction of the letter *e* into those Hermann–Mauguin symbols where a couple of the symbols *a*, *b*, *c* has an equivalent meaning and with the introduction of dash–double-dotted lines in the corresponding diagrams.

Consideration of magnetic properties and of crystals with atoms (or ions) that carry magnetic momentum requires the introduction of magnetic point and space groups. The magnetic point groups are sometimes called Heesch groups because they were derived by Heesch in 1930 as the three-dimensional groups of four-dimensional space. In the older Russian literature, we can also find another system of symbols for point and space groups developed by Shubnikov. These symbols were also introduced for magnetic groups and the magnetic space groups are also called Shubnikov groups, mostly again in the Russian literature. At the moment, we can say that these symbols have generally been abandoned. We shall therefore adopt the position that there is a common consensus to use only the Schoenflies and Hermann–Mauguin symbols for the description of point and space groups, including the magnetic groups.

These groups, however, do not exhaust all groups of interest in materials physics or even all groups which deserve to be called ‘crystallographic groups’. There exist chemical compounds with symmetries that are not crystallographic and in the solid state so-called quasicrystals were found to form and their description requires non-crystallographic groups. Since in general molecules have no periodicity, their symmetries are usually called *point groups*. Moreover, the application of group theory is not limited to the description of structures and the most powerful uses of groups lie in applications of the theory of group representations.

The *International Tables for Crystallography* were prepared by crystallographers and consequently reflect the exigencies of the practical determination and description of crystal structures. Space groups therefore describe symmetries of possible structures in the model of so-called *ideal crystals*, which means monocrystals that fill the whole space, so that surface effects can be neglected. However, crystalline materials frequently consist of monocrystals of various orientations, there exists a phenomenon called *twinning* in which two monocrystals of different orientations join along a certain plane and, finally, in structural phase transitions there appear regions of low symmetry, called *domains*, whose structures are, in a given transition, identical up to orientation and shift in space. Consideration of boundaries now constitutes a subject which is known under the name of *bicrystallography* (Pond & Vlachavas, 1983). Symmetries of domain walls and twin boundaries are described by groups of two-dimensional periodicity which are known under the name *layer groups*. Symmetries of linear edifices in a crystal are accordingly described by groups with one-dimensional periodicity known now under the name *rod groups*.

Both types of these groups have been historically derived and rederived under different names since the first decades of the last century and various symbols were invented for their classification. Eventually, in a manner analogous to the standards for space groups, standards for these groups were introduced in *International Tables for Crystallography* (2002), Vol. E, *Subperiodic Groups* (abbreviated here as *ITE*). Comparative tables, given in this volume, of symbols used at various times by different authors show that at least 9 types of

symbols for frieze groups, 6 for rod groups and 20 for layer groups have been used. Hermann–Mauguin types of symbols for layer groups were introduced and tables analogous to those for the space groups were derived by Wood (1964). Our notation is, however, closer to that introduced by Bohm & Dornberger-Schiff (1966, 1967), used also later in tables by Grell *et al.* (1989). The reason for this choice lies in the background of the *unified system of Hermann–Mauguin symbols* which is based on the fact that subperiodic groups are isomorphic to factor groups of *reducible space groups* (Kopský, 1986, 1988*b*, 1989*a,b*, 1993*a*; Fuksa & Kopský, 1993; see also §5).

Both volumes A and E of the *International Tables for Crystallography* are restricted to the description of only those groups of isometries that are crystallographic and whose translation subgroups are discrete. On the other hand, problems of material physics involve groups with continuous or semicontinuous translation subgroups (lattices in crystallographic terminology) as well as groups of non-crystallographic character. Although ideal crystals always have discrete lattices, it is sometimes suitable to neglect their microscopic structure and consider them as continuous media. Such an approximation is used, for example, in the consideration of ‘ferroic’ phase transitions. In this case, it is appropriate to consider the symmetry as a group whose lattice is continuous. In the consideration of domain walls or twin boundaries in the same approximation, we need to consider layer groups whose lattices are also continuous. In this connection, it is necessary to amend the usual meaning of terms *crystallographic* and *space groups* (see §3). We shall consider here all cases in which the point and translation subgroups are discrete, semicontinuous or continuous. The site point groups and point groups will be considered in more detail in the accompanying papers on tensor calculus (Kopský, 2006*a,b*).

## 2. The elementary theory of Euclidean groups

The fact that the universe in the nonrelativistic approximation is a three-dimensional point space  $E(3)$  of Euclidean type is established by experiment. We shall consider elementary properties of such spaces for arbitrary dimensions. An Euclidean space  $E(n)$  of dimension  $n$  is a point space on which there is defined an Euclidean metric and hence also the orthogonality of directions. As a result, this space is associated with a vector space  $V(n)$  of dimension  $n$  on which there is defined a scalar product  $(\mathbf{a}, \mathbf{b})$  of any of its two vectors  $\mathbf{a}$ ,  $\mathbf{b}$  and hence the norm of a vector  $|\mathbf{x}| = (\mathbf{x}, \mathbf{x})^{1/2}$ . In the space  $V(n)$ , we can choose an orthonormal basis  $\{\mathbf{e}_i\}_{i=1}^n$  so that  $(\mathbf{e}_i, \mathbf{e}_j) = \delta_{ij}$ , where  $\delta_{ij}$ , known as the Kronecker delta, equals 1 only if  $i = j$  and zero otherwise. Vectors satisfying these conditions are linearly independent and their number  $n$  defines the dimension of the space  $V(n)$ , so that each vector  $\mathbf{x}$  of  $V(n)$  may be expressed as

$$\mathbf{x} = \sum_{i=1}^n x_i \mathbf{e}_i, \quad \text{and the scalar product is } (\mathbf{a}, \mathbf{b}) = \sum_{i=1}^n a_i b_i,$$

where  $\mathbf{a} = \sum_{i=1}^n a_i \mathbf{e}_i$ ,  $\mathbf{b} = \sum_{i=1}^n b_i \mathbf{e}_i$ . The norm of a vector is then expressed by  $|\mathbf{x}| = (\sum_{i=1}^n x_i^2)^{1/2}$ .

The space  $V(n)$  is usually called the *difference space* of  $E(n)$ . Each of its vectors  $\mathbf{x}$  corresponds to infinitely many pairs of points  $X_1, X_2 \in E(n)$  which is written formally as  $\mathbf{x} = X_2 - X_1$  and the norm of vector  $|\mathbf{x}| = [(\sum_{i=1}^n (x_{2i} - x_{1i})^2)^{1/2}]$  is equal to the distance between any pair of these points.

A mapping  $g : V(n) \rightarrow V(n)$  of the space  $V(n)$  onto itself (a bijection) or onto one of its proper subspaces (an injection) is called *linear* if

$$g(\mathbf{ax} + \mathbf{by}) = \mathbf{a}g\mathbf{x} + \mathbf{b}g\mathbf{y}.$$

Mappings on a proper subspace are also called *projections*. Bijections satisfy the condition that to each bijection  $g$  there exists its inverse  $g^{-1}$ , so that, if  $g$  maps an arbitrary vector  $\mathbf{x} \in V(n)$  onto a vector  $\mathbf{y} = g\mathbf{x}$ , then  $g^{-1}$  maps the vector  $\mathbf{y}$  onto  $\mathbf{x} = g^{-1}\mathbf{y} = g^{-1}g\mathbf{x}$ . Hence the mapping  $g^{-1}g$  and  $gg^{-1}$  is also the identity mapping which maps each vector  $\mathbf{x} \in V(n)$  onto itself. This mapping will be denoted by  $e$ . All bijections form a group  $\mathcal{GV}(n)$ , called the *general linear group* on  $V(n)$ .

A linear mapping  $g : V(n) \rightarrow V(n)$  is called *orthogonal* if it leaves scalar products invariant so that  $(g\mathbf{a}, g\mathbf{b}) = (\mathbf{a}, \mathbf{b})$  for each pair of vectors  $\mathbf{a}, \mathbf{b}$ . All orthogonal transformations constitute a group  $\mathcal{O}(n)$ , called the *orthogonal group* of dimension  $n$  which is a subgroup of  $\mathcal{GV}(n)$ . Mapping can be interpreted either as a transformation of bases or as a linear or orthogonal operator on  $V(n)$ . Orthogonal mappings send the orthonormal bases back into orthonormal bases because they do not change the scalar products. Linear mappings can be expressed by  $n \times n$  matrices according to

$$g\mathbf{e}_i = \sum_{j=1}^n D_{ji}(g)\mathbf{e}_j.$$

Thus the choice of a basis  $\{\mathbf{e}_i\}_{i=1}^n$  defines an isomorphism of the group  $\mathcal{GV}(n)$  with the group  $GL(n; R)$  of real invertible matrices called the *general linear group (of  $n$ -dimensional matrices)* and of the group  $\mathcal{O}(n)$  with the group  $\mathcal{O}(n)$  of matrices which are orthogonal if and only if the vectors of the basis  $\{\mathbf{e}_i\}_{i=1}^n$  are mutually orthogonal.

*Euclidean spaces:* Any point  $X$  of an Euclidean space  $E(n)$  can be expressed as a certain chosen point  $P$ , called the *origin* plus a vector  $\mathbf{x} \in V(n)$ . The origin together with the basis of  $V(n)$  constitute a *coordinate system*  $(P; \{\mathbf{e}_i\}_{i=1}^n)$ . Any point  $X \in E(n)$  is then formally expressed as  $X = P + \mathbf{x}$ . The set of values  $(x_1, x_2, \dots, x_n)$  is interpreted either as the set of components of a vector  $\mathbf{x}$  in the basis  $\{\mathbf{e}_i\}_{i=1}^n$  or as a set of coordinates of a point  $X$  in the coordinate system  $(P; \{\mathbf{e}_i\}_{i=1}^n)$ .

### 2.1. Isometries and Seitz symbols

A mapping of an Euclidean space  $E(n)$  onto itself is called an *isometry (rigid motion or Euclidean transformation)* if it leaves the distances between points invariant. We distinguish two kinds of basic transformations.

1. Rotation of the space  $E(n)$  about a chosen point  $P$ . To each rotation there corresponds an element  $g \in \mathcal{O}(n)$  such that the action of the rotation on the point  $P + \mathbf{x}$  is expressed by  $P + g\mathbf{x}$ . All rotations about an arbitrary point  $P$  then constitute a group  $\mathcal{O}_P(n)$  of all isometries which leave the point  $P$  invariant. Each such group is isomorphic with the orthogonal group  $\mathcal{O}(n)$ .

We distinguish proper rotations that have the property that their matrices  $D(g)$  have determinant  $|D(g)| = 1$  from improper rotations whose matrices have determinant  $|D(g)| = -1$ . Proper rotations constitute a halving subgroup of  $\mathcal{O}(n)$ , denoted by  $\mathcal{SO}(n)$  and called the *special orthogonal group*. Improper rotations constitute a coset  $m\mathcal{SO}(n)$ , where  $m$  is any element with  $|D(m)| = -1$ . It is, however, suitable to consider as  $m$  that element of  $\mathcal{O}(n)$  to which there corresponds a hyperplane in  $E(n)$ . The matrix of such an element in a suitable basis is diagonal with all entries on the diagonal being 1 except one which is  $-1$ .

*Remark.* A space inversion, denoted by  $i$ , changes the sign of any vector and hence its matrix  $D(i) = -I$ , the negative of unit matrix  $I$  in any coordinate system. If  $n$  is even, then  $i \in \mathcal{SO}(n)$  is a proper rotation; if  $n$  is odd, then  $i \in m\mathcal{SO}(n)$  is an improper rotation.

2. Translation of the whole space by a certain vector  $\mathbf{t} \in V(n)$ . This isometry sends any point  $Q \in E(n)$  to the point  $Q + \mathbf{t}$ . The following lemma, formulated here without proof, is the starting point of the theory of Euclidean groups.

*Lemma 1.* Any isometry can be expressed as a result of a certain rotation of the space about any chosen point  $P$  followed by a certain translation.

*Seitz symbols:* In view of this lemma, we introduce the symbols of isometries which bear the name of Seitz. Such a symbol, for an isometry that consists of a rotation  $g$  about a point  $P$  followed by translation  $\mathbf{t}$  is denoted by  $\{g|\mathbf{t}\}_P$  and it acts on the point  $X = P + \mathbf{x}$  as follows:

$$\{g|\mathbf{t}\}_P(P + \mathbf{x}) = P + g\mathbf{x} + \mathbf{t}.$$

All isometries constitute the *full Euclidean group* in  $n$  dimensions, which we denote by  $\mathcal{E}(n)$ . The multiplication law on this group has the form

$$\{g|\mathbf{t}_g\}_P\{h|\mathbf{t}_h\}_P = \{gh|\mathbf{t}_g + g\mathbf{t}_h\}_P,$$

the unit of the group  $\mathcal{E}(n)$  is

$$\{e|\mathbf{0}\}_P$$

and the reciprocal to an element  $\{g|\mathbf{t}\}_P$  is

$$\{g|\mathbf{t}_g\}_P^{-1} = \{g^{-1}|\mathbf{t}_g - g^{-1}\mathbf{t}_g\}_P.$$

If we change the reference point  $P$  (the origin) to the point  $Q = P + \mathbf{s}$ , then the point  $X$  is expressed as  $X = Q + \mathbf{x} - \mathbf{s}$  and

$$\begin{aligned} \{g|\mathbf{t}\}_Q X &= \{g|\mathbf{t}\}_Q(Q + \mathbf{x} - \mathbf{s}) = Q + g\mathbf{x} - g\mathbf{s} + \mathbf{t} \\ &= P + g\mathbf{x} + \mathbf{s} - g\mathbf{s} + \mathbf{t} = \{g|\mathbf{t} + \varphi(g, \mathbf{s})\}_P X, \end{aligned}$$

where

$$\varphi(g, \mathbf{s}) = \mathbf{s} - g\mathbf{s}$$

is a so-called *shift function*. Since the relation holds for any  $X$ , we obtain that

$$\{g|\mathbf{t}\}_{P+\mathbf{s}} = \{g|\mathbf{t} + \varphi(g, \mathbf{s})\}_P$$

and, conversely,

$$\{g|\mathbf{t}\}_P = \{g|\mathbf{t} - \varphi(g, \mathbf{s})\}_{P+\mathbf{s}}.$$

The first of these relations shows how an isometry that operates in a certain manner with reference to point  $Q = P + \mathbf{s}$  is expressed by a Seitz symbol with reference to point  $P$ . The second relation shows how the Seitz symbol for a certain isometry, expressed with reference to a point  $P$ , changes if we express it with reference to a point  $Q = P + \mathbf{s}$ .

The subscript  $P$ , referring to the origin, is usually dropped in most textbooks on the assumption that the origin is fixed. In our consideration, the distinction of Seitz symbols with reference to different origins is essential.

*Geometric interpretation and location properties of isometries:* We consider now an element  $g \in \mathcal{O}(n)$ . The space  $V(n)$  splits under the action of  $g$  into two mutually orthogonal subspaces:  $V(n) = V_f(g) \oplus V_l(g)$ , where  $V_f(g)$  is defined as that subspace of  $V(n)$  which contains all vectors  $\mathbf{s}$  for which  $\varphi(g, \mathbf{s}) = 0$ . In other words, this space contains all translations which are invariant under the action of  $g$ , so that  $g\mathbf{s} = \mathbf{s}$ . The space  $V_l(g)$  is chosen as an orthogonal complement of  $V_f(g)$ .

To the element  $g \in \mathcal{O}(n)$ , there correspond infinitely many elements  $\{g|\mathbf{t}\}_P \in \mathcal{E}(n)$ . We split the translation  $\mathbf{t}$  into its components  $\mathbf{t}_f \in V_f(g)$  and  $\mathbf{t}_l \in V_l(g)$ , so that  $\mathbf{t} = \mathbf{t}_f + \mathbf{t}_l$  and express the element  $\{g|\mathbf{t}\}_P$  with reference to another point  $P + \mathbf{s}$ , so that

$$\{g|\mathbf{t}\}_P = \{g|\mathbf{t} - \varphi(g, \mathbf{s})\}_{P+\mathbf{s}} = \{g|\mathbf{t}_f + \mathbf{t}_l - \varphi(g, \mathbf{s})\}_{P+\mathbf{s}}.$$

If we also split the vector  $\mathbf{s} = \mathbf{s}_f + \mathbf{s}_l$  into its components  $\mathbf{s}_f \in V_f(g)$  and  $\mathbf{s}_l \in V_l(g)$ , we find that  $\varphi(g, \mathbf{s}) = \varphi(g, \mathbf{s}_l)$  because  $g\mathbf{s}_f = \mathbf{s}_f$ , so that  $\varphi(g, \mathbf{s}_f) = \mathbf{0}$  and

$$\{g|\mathbf{t}\}_P = \{g|\mathbf{t}_f + \mathbf{t}_l - \varphi(g, \mathbf{s}_l)\}_{P+\mathbf{s}}.$$

The equation  $\mathbf{t}_l - \varphi(g, \mathbf{s}_l) = \mathbf{0}$  always has a solution  $\mathbf{s}_l$  for which

$$\{g|\mathbf{t}\}_P = \{g|\mathbf{t}_f\}_{P+\mathbf{s}_l}.$$

From this result, we reach two conclusions:

(i) the shift of origin by any  $\mathbf{s}_f \in V_f(g)$  does not change the element  $\{g|\mathbf{t}\}_P$ , and

(ii) we can find an origin  $P + \mathbf{s}_l$  for which  $\{g|\mathbf{t}\}_P = \{g|\mathbf{t}_f\}_{P+\mathbf{s}_l}$ .

From this follows a geometrical description of the action of an element  $\{g|\mathbf{t}\}_P$  on  $E(n)$ . The action of this element on the subspace  $(P + \mathbf{s}_l; V_f(g))$  is reduced to a translation  $\mathbf{t}_f$ . In the three-dimensional case, this subspace can be a point  $P + \mathbf{s}_l$ , a line or a plane passing through this point, or the whole space. In the first case,  $V_f(g) = V(3)$ , the only allowed translation is

$\mathbf{t}_f = \mathbf{0}$  and the element  $\{g|\mathbf{t}\}_P = \{g|\mathbf{0}\}_{P+\mathbf{s}_l}$  leaves the point  $P + \mathbf{s}_l$  invariant. Such elements are either the inversion or rotoinversion at the point  $P + \mathbf{s}_l$ . For  $V_f(g)$  one- or two-dimensional, we obtain either screw axes or glide planes where  $\mathbf{t}_f$  are the screw or glide translations (if this vector is trivial, we obtain an ordinary axis or plane). In higher dimensions, we obtain analogously higher-dimensional subspaces. Finally, the case when  $V_f(n) = V(n)$  corresponds to  $g = e$  in any dimension and the element is simply a translation  $\{e|\mathbf{t}\}$ . In this particular case, it is not at all necessary to specify the origin  $P$  in the Seitz symbol.

Finally, let us comment on the choice of subscripts  $f$  and  $l$  which stand for the verbal description of an element  $\{g|\mathbf{t}\}_P$  as ‘floating’ in  $(P + \mathbf{s}_l; V_f(g))$  and ‘localized’ in any of the point spaces  $(P + \mathbf{s}_f; V_l(g))$ .

The vector space  $V(n)$  appears in these considerations in two roles.

(i) As the space of all translations  $\{e|\mathbf{t}\}$ . In this role, the space  $V(n)$  is the subgroup of the full Euclidean group  $\mathcal{E}(n)$ .

(ii) As the space of difference vectors  $\mathbf{x}$  on which the elements of  $\mathcal{O}(n)$  act.

*Lemma 2.* As a subgroup of  $\mathcal{E}(n)$ , the space  $V(n)$  is its normal subgroup. Indeed, any conjugate element to a translation  $\{e|\mathbf{t}\} \in V(n)$  can be expressed as

$$\{g|\mathbf{t}_g\}_P \{e|\mathbf{t}\} \{g^{-1}|\mathbf{t}_g^{-1}\}_P = \{e|g\mathbf{t}\} \in V(n).$$

According to the theory of normal subgroups, there exists a homomorphism that maps the group  $\mathcal{E}(n)$  onto the factor group  $\mathcal{E}(n)/V(n)$  whose unit element  $V(n)$  contains all translations  $\{e|\mathbf{t}\}$  and cosets contain all elements  $\{g|\mathbf{t}\}_P$  with the same  $g$  (the change of  $P$  does not change  $g$ ). Choosing coset representatives as  $\{g|\mathbf{t}\}_P$ , we obtain those homomorphisms  $\sigma_P : \mathcal{E}(n) \rightarrow \mathcal{O}_P(n)$  of  $\mathcal{E}(n)$  that map  $\mathcal{E}(n)$  onto groups of rotations about any chosen point  $P$ . We introduce the homomorphism  $\sigma : \mathcal{E}(n) \rightarrow \mathcal{O}(n)$ , which maps each element  $\{g|\mathbf{t}\}_P \in \mathcal{E}(n)$  onto its orthogonal part  $g \in \mathcal{O}(n)$ , so that  $\sigma(\{g|\mathbf{t}\}_P) = g$ . It is  $\text{Ker } \sigma(\mathcal{E}(n)) = V(n)$  and  $\text{Im } \sigma(\mathcal{E}(n)) = \mathcal{O}(n)$ .

*Remark.* An affine transformation of  $E(n)$  is, by definition, any transformation that leaves parallel subspaces parallel. The group  $\mathcal{A}(n)$  of all affine transformations of  $E(n)$  contains the group of Euclidean transformations as its subgroup. Generally, an affine transformation can be expressed again by Seitz symbol  $\{g|\mathbf{t}\}_P$ , where  $g \in \mathcal{G}V(n)$ .

## 2.2. The fundamental theorem on Euclidean groups

The group  $\mathcal{E}(n)$  is called the *full Euclidean group of dimension  $n$*  and its subgroups are called *Euclidean groups* (of dimension  $n$ ). We shall formulate now without proof a theorem for the Euclidean groups though an analogous theorem holds also for the affine groups.



*Theorem 1. (Fundamental theorem on Euclidean groups).* Every Euclidean group can be expressed by a symbol

$$\mathcal{G} = \{G, T_G, P, \mathbf{u}_G(g)\} = \{G, T_G, P + \mathbf{s}, \mathbf{u}_G(g) - \varphi(g, \mathbf{s})\},$$

which has the meaning of the set of all isometries of the form  $\{g|\mathbf{t} + \mathbf{u}_G(g)\}_P = \{g|\mathbf{t} + \mathbf{u}_G(g) - \varphi(g, \mathbf{s})\}_{P+\mathbf{s}}$ , where the symbols are defined as follows.

(i)  $g$  are elements of a group  $G \subseteq \mathcal{O}(n)$  acting on the vector space  $V(n)$  – this is the so-called ‘point group’ of the Euclidean group  $\mathcal{G}$  and it is  $\sigma(\mathcal{G}) = G = \text{Im } \sigma(\mathcal{G})$ .

(ii)  $T_G$  is a  $G$ -invariant subgroup of  $V(n)$ , which contains all translations  $\mathbf{t}$  present in the elements of  $\mathcal{G}$ . It is therefore  $GT_G = T_G$ , and  $T_G \triangleleft \mathcal{G}$  (the symbol  $\triangleleft$  means normal subgroup). This is the *translation subgroup* or, in crystallographic language, the *vector lattice* of the group  $\mathcal{G}$  and it is evidently  $T_G = \mathcal{G} \cap V(n) = \text{Ker } \sigma(\mathcal{G})$  and  $G \approx \mathcal{G}/T_G$ .

(iii)  $\mathbf{u}_G : g \rightarrow \mathbf{u}_G(g) \in V(n)$  is a function that satisfies the so-called Frobenius congruences:

$$\mathbf{w}_G(g, h) = \mathbf{u}_G(g) + g\mathbf{u}_G(h) - \mathbf{u}_G(gh) = \mathbf{0} \pmod{T_G}$$

or, equivalently,

$$\mathbf{w}_G(g, h) \in T_G \quad \text{for every pair of } g, h \in G.$$

In particular, for the full Euclidean group we have

$$\mathcal{E}(n) = \{\mathcal{O}(n), V(n), P, \mathbf{u}_G(g) \equiv \mathbf{0}\}.$$

The functions  $\mathbf{u}_G(g)$  are known as the *systems of non-primitive translations*, the functions  $\mathbf{w}_G(g, h)$  as the *factor systems*. The systems of non-primitive translations for the same group with reference to different origins  $P$  differ by a shift function  $\varphi(g, \mathbf{s})$ . Quite generally, any function  $\mathbf{u}_G(g) : G \rightarrow V(n)$ , which satisfies the Frobenius congruences, defines a group  $\mathcal{G}$ . If  $\mathbf{u}_G(g)$  has this property, then the function  $\mathbf{u}_G(g) + \mathbf{t}_G(g)$ , where  $\mathbf{t}_G(g) : G \rightarrow T_G$  also has it and defines the same group  $\mathcal{G}$ . To achieve uniqueness of the relationship between groups and systems of non-primitive translations, we therefore restrict  $\mathbf{u}_G(g)$  to the fundamental region  $[V(n)/T_G]$  of  $T_G$ . This region contains representatives of coset resolution of the space  $V(n)$ , considered as an Abelian group, with respect to its subgroup  $T_G$ . In the Euclidean space  $E(n)$ , there corresponds to it the fundamental region of the translation group  $T_G$  which can be chosen in infinitely many ways. It is usual to choose it either as a Wigner–Seitz cell or as the unit cell. We shall always use the latter choice.

*The location properties of Euclidean groups:* In Theorem 1, we expressed the same group  $\mathcal{G}$  with reference to different origins of the coordinate system. On the other hand, the group  $\mathcal{G}(\mathbf{s})$  defined by

$$\mathcal{G}(\mathbf{s}) = \{G, T_G, P + \mathbf{s}, \mathbf{u}_G(g)\} = \{G, T_G, P, \mathbf{u}_G(g) + \varphi(g, \mathbf{s})\}$$

has evidently the meaning of a group of isometries which acts on  $E(n)$  in the same manner with reference to the origin  $P + \mathbf{s}$  as the group  $G$  acts with reference to the origin  $P$ .

*Proposal:* In connection with this relation, we suggest the location of Euclidean groups be described as follows. (i) Assign to each Hermann–Mauguin symbol a certain standard

location of the group in space. In crystallographic language, this corresponds to the choice of origin. Thus, if  $\mathcal{G}$  is a certain Hermann–Mauguin symbol, there exists one and only one diagram which describes the group. (ii) If the location of the group (choice of origin) differs from the standard, write the shift in parentheses after the standard Hermann–Mauguin symbol, *i.e.* write it exactly as  $\mathcal{G}(\mathbf{s})$ .

Let us observe that we used this principle in defining the standards of subperiodic groups in *ITE* and to interpret the Hermann–Mauguin symbols from *ITA*. This was necessitated by the Scanning Tables in which the location of space groups as well as their sectional layer groups are of prime importance.

*Translation normalizers:* Inspecting diagrams of space or of subperiodic groups, we can see that certain translations do not change them. These translations  $\mathbf{s}$  are those which satisfy the relation  $\varphi(g, \mathbf{s}) = \mathbf{s} - g\mathbf{s} \in T_G$ . These translations constitute a group called the *translation normalizer* of the group  $\mathcal{G}$ , denoted by  $T_N(\mathcal{G})$ , and they are common to all groups with the same pair  $(G, T_G)$ . Such a set of groups constitutes an *oriented arithmetic class with fixed parameters* (*cf.* next section). Translation normalizers were considered by Kopský (1993*b,c*) and they represent the translation subgroups of the Euclidean normalizers given in *ITA*.

Systems of non-primitive translations, factor systems and shift functions appear in two very exacting papers by Ascher & Janner (1965, 1968/69) on space groups in arbitrary dimensions in which the theory of space groups in arbitrary dimensions is treated on the basis of the theory of *cohomology groups*. Our approach is a plain extension of this theory to subperiodic and other Euclidean groups. The author wishes to acknowledge a series of lectures given by the recognized Czech specialist on Abelian groups, Professor L. Procházka from Charles University in Prague, who helped a small group of our theorists to decipher these papers. It might be worth mentioning that he was happy to find that such an exacting theory has practical application in crystallography.

### 2.3. The fundamental theorem on arithmetic classes

We shall now consider Euclidean groups with the same pair  $(G, T_G)$  of the point group  $G$  and of the translation subgroup (lattice)  $T_G$ . The set of all such distinct groups constitutes an oriented arithmetic class with fixed parameters, *i.e.* groups with the same orientation of the point group  $G$  and with the same parameters which define the translation subgroup  $T_G$ . All groups of the *arithmetic class* are obtained by applying admissible affine transformations; the whole set of groups of the arithmetic class will contain Euclidean groups of oriented arithmetic classes with fixed parameters  $(\alpha G \alpha^{-1}, \alpha T_G)$  (the orientation refers to both  $G$  and  $T_G$  while  $T_G$  still has free parameters). Whatever we say about groups with the same pair  $(G, T_G)$  can then be applied to groups with pairs  $(\alpha G \alpha^{-1}, \alpha T_G)$ .

Furthermore, if  $\mathcal{G} = \{G, T_G, P, \mathbf{u}_G(g)\}$  is a certain Euclidean group, then the group

$$\mathcal{G}(\mathbf{s}) = \{G, T_G, P + \mathbf{s}, \mathbf{u}_G(g)\} = \{G, T_G, P, \mathbf{u}_G(g) + \varphi(g, \mathbf{s})\}$$

is related to the origin  $P + \mathbf{s}$  in exactly the same way as the group  $\mathcal{G}$  is related to the origin  $P$ . It is  $\mathcal{G} = \mathcal{G}(\mathbf{s})$  if  $\varphi(g, \mathbf{s}) \in T_G$ , which means that  $\mathbf{s}$  is an element of the translation normalizer  $T_N(\mathcal{G}) = T_N(G, T_G)$ . The last expression refers to the fact that all groups of the same oriented arithmetic class  $(G, T_G)$  with fixed parameters have the same translation normalizer which reflects their location properties (Kopský, 1993bc). Each group  $\mathcal{G}(\mathbf{s})$  is therefore represented if  $\mathbf{s}$  runs through the fundamental region  $[V(n)/T_N(G, T_G)]$ .

*Theorem 2. (Fundamental theorem on arithmetic classes).* Every group of the oriented arithmetic class  $(G, T_G)$  with fixed parameters can be expressed as

$$\mathcal{G}^{(\alpha)}(\mathbf{s}) = \{G, T_G, P + \mathbf{s}, \mathbf{u}_G^{(\alpha)}(g)\} = \{G, T_G, P, \mathbf{u}_G^{(\alpha)}(g) + \varphi(g, \mathbf{s})\}$$

and the set of the systems of non-primitive translations  $\mathbf{u}_G^{(\alpha)}$  can be chosen so that it forms an additive group.

*Baer multiplication:* It is therefore possible to introduce a formal multiplication of the symbols of Euclidean groups of the same arithmetic class:

$$\mathcal{G}^{(\alpha)}(\mathbf{s}_1) \circ \mathcal{G}^{(\beta)}(\mathbf{s}_2) = \mathcal{G}^{(\gamma)}(\mathbf{s}_1 + \mathbf{s}_2),$$

which corresponds to

$$\mathbf{u}_G^{(\alpha)}(g) + \varphi(g, \mathbf{s}_1) + \mathbf{u}_G^{(\beta)}(g) + \varphi(g, \mathbf{s}_2) = \mathbf{u}_G^{(\gamma)}(g) + \varphi(g, \mathbf{s}_1 + \mathbf{s}_2).$$

We name this law after Baer (1934, 1949), the great contributor to the theory of group extensions from which all cohomology considerations stem. It is a check that all systems of non-primitive translations  $\mathbf{u}_G^{(\alpha)}(g) + \varphi(g, \mathbf{s})$  result in the same factor system  $\mathbf{w}_G^{(\alpha)}(g, h)$ .

*Remark.* The trivial system of non-primitive translations  $\mathbf{u}_G^{(\alpha)}(g) \approx \mathbf{0}$  corresponds to the symmorphic group of the class  $(G, T_G)$  with origin at the point of the symmetry  $G$ .

*Application to space groups:* The concept of arithmetic classes has been introduced for space groups and here it is extended to all Euclidean groups. Let us see what conclusions we can make so far for the classical space groups. According to definition, the point group  $G$  defines the *oriented geometric class* to which the space group  $\mathcal{G}$  belongs. Conjugate groups  $hGh^{-1}$  define other oriented geometric classes all of which constitute the *geometric class* of space groups. The pair  $(G, T_G)$  defines an *oriented arithmetic class with fixed parameters*. In terms of space-group diagrams that visualize the group, the parameters of  $T_G$ , which are the vectors  $(\mathbf{a}, \mathbf{b}, \mathbf{c})$  of the crystallographic basis, define the frame in which we draw the diagram. Each system of non-primitive translations  $\mathbf{u}_G^{(\alpha)}(g)$  defines a certain space group  $\mathcal{G}^{(\alpha)}$  and hence a certain diagram. The group  $\mathcal{G}^{(\alpha)}(\mathbf{s})$  has the same diagram, shifted by  $\mathbf{s}$  in the reference frame. If  $\mathbf{s}$  is in the translation normalizer, the diagram coincides with the original. Taking all systems of non-primitive translations  $\mathbf{u}_G^{(\alpha)}(g)$  and all shifts  $\mathbf{s} \in [V(n)/T_N(G, T_G)]$ , we exhaust all groups of the oriented

arithmetic class  $(G, T_G)$  and hence also all diagrams that fit the frame. Groups with different labels  $\alpha, \beta$  are not necessarily of a different space-group type.

*Addendum to the proposal:* The label  $\alpha$  of the system of non-primitive translations defines the diagram of the space group up to its location (choice of origin) uniquely. The majority of diagrams of space groups in *ITA* (all diagrams in *ITE*) are associated uniquely with Hermann–Mauguin symbols. These symbols are missing from the diagrams of the monoclinic space groups but they can easily be deduced. From this viewpoint, the symbol  $Pb\bar{3}$  is also missing from the diagram of the group type  $T_h^6$ .

There are therefore three ways to characterize a space group uniquely with reference to a crystallographic basis:

- (i) by the label  $\alpha$  of the system of non-primitive translations and by the shift  $\mathbf{s}$ ;
- (ii) by the Hermann–Mauguin symbol with shift  $\mathbf{s}$  behind it, provided that a correspondence of zero shift with a certain system of non-primitive translations be established;
- (iii) by its diagram.

### 3. Reducibility and decomposability of Euclidean groups

In most textbooks on applications of group theory to atomic or solid-state physics, the concepts of reducibility and decomposability are not distinguished. We shall briefly explain the difference and why we need to distinguish these two cases.

*Definition 3.1.* Let a group  $G$  act on a linear space  $V(n)$ . We say that this action (or that the group  $G$ ) is *reducible* if there exists a proper subspace  $V(k)$  of  $V(n)$  which is invariant under the action of  $G$ , so that  $g\mathbf{x} \in V(k)$  for all  $g \in G$  if  $\mathbf{x} \in V(k)$ . We say that the action of  $G$  on  $V(n)$  is *decomposable* if the space  $V(n)$  splits into a direct sum of proper subspaces  $V(n) = V(k_1) \oplus V(k_2)$  both of which are invariant under the action of  $G$ .

In terms of matrix representations of these groups, this means that all matrices  $D(g)$  for  $g \in G$  can be, by a suitable choice of basis, brought to either of the forms

$$D(g) = \begin{pmatrix} D_1(g) & 0 \\ D_{12}(g) & D_2(g) \end{pmatrix} \quad \text{or} \quad \begin{pmatrix} D_1(g) & 0 \\ 0 & D_2(g) \end{pmatrix},$$

where the first corresponds to reducibility, the second to decomposability.

For the groups we consider in material physics, reducibility implies decomposability when action on linear spaces is considered so that there is no need to distinguish them. However, in our consideration of arithmetic classes  $(G, T_G)$ , the group  $G$  acts on  $T_G$  which need not be a linear space. In the case of space groups in their usual meaning, which will be later amended, their translation subgroups (lattices)  $T_G$  are discrete subgroups of  $V(n)$ . In proper algebraic language, such

structures are called *modules*. We shall briefly describe the difference between linear spaces and modules.

A linear (vector) space contains linear combinations  $a_1\mathbf{x}_1 + a_2\mathbf{x}_2 + \dots + a_m\mathbf{x}_n$  of any set of its vectors  $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n$  with coefficients  $a_i$  from a number field. The term field means that the ratio  $a/b$  of two numbers is defined unless  $b = 0$ . This enables us to define linear independence and the number of linearly independent vectors  $\mathbf{x}_i$  whose linear combinations represent all vectors of the space is called the *dimension* of this space and a set of these vectors is called a *basis*. It is a substantial property of linear spaces that each set of linearly independent vectors whose number equals the dimension is a basis. In our applications, we need only the fields  $Q$  of rationals,  $R$  of real numbers and  $C$  of complex numbers.

A module also contains a linear combination  $n_1\mathbf{x}_1 + n_2\mathbf{x}_2 + \dots + n_m\mathbf{x}_n$  of any set of its vectors  $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n$  with coefficients  $n_i$  from a *ring* such as the set  $Z$  of integers. The set of vectors whose linear combinations with coefficients from the ring exhaust all vectors of the module is again called its basis. Their number is called the *rank* of the module. However, in a ring the ratio of two numbers does not exist for an arbitrary pair (the ratio  $n/m$  of two integers  $n, m \in Z$  belongs to the ring  $Z$  if and only if  $m$  is a divisor of  $n$ ). As a result, there exist sets of linearly independent vectors in a module that do not form a basis although their number equals the rank.

We shall now briefly describe what this means in three-dimensional space. Let us consider the conventional crystallographic basis  $(\mathbf{a}, \mathbf{b}, \mathbf{c})$  of a certain space group. We denote by  $T(\mathbf{a}, \mathbf{b}, \mathbf{c})$  the set of all vectors of the form  $\mathbf{t} = n_1\mathbf{a} + n_2\mathbf{b} + n_3\mathbf{c}$ , where  $n_1, n_2, n_3$  are integers. The set of vectors  $(2\mathbf{a}, \mathbf{b}, \mathbf{c})$  evidently is not a basis of  $T(\mathbf{a}, \mathbf{b}, \mathbf{c})$ . Actually, if we consider a centred lattice, then the conventional basis is not even a basis of the lattice in its algebraic meaning. The space  $V(3)$  contains all vectors of the form  $\mathbf{x} = x\mathbf{a} + y\mathbf{b} + z\mathbf{c}$ , where  $x, y, z$  are real numbers. With the exception of cubic groups, the action of point groups of all space groups on  $V(\mathbf{a}, \mathbf{b}, \mathbf{c})$  is reducible and also decomposable because the space splits into a direct sum  $V(\mathbf{a}, \mathbf{b}) \oplus V(\mathbf{c})$  in cases of a standard orientation of a point group  $G$  for all groups with the exception of the cubic system. If we now consider those vectors of the lattice  $T_G$  which are elements of subspaces  $V(\mathbf{a}, \mathbf{b})$ ,  $V(\mathbf{c})$ , we obtain a two-dimensional lattice  $T_{G1} = T_G \cap V(\mathbf{a}, \mathbf{b}) = T(\mathbf{a}, \mathbf{b})$  and a one-dimensional lattice  $T_{G2} = T_G \cap V(\mathbf{c}) = T(\mathbf{c})$ . If the lattice  $T_G$  is primitive, it is identical with the direct sum  $T_{G1} \oplus T_{G2} = T(\mathbf{a}, \mathbf{b}) \oplus T(\mathbf{c})$ . This is also true if the centring vector lies in the space  $V(\mathbf{a}, \mathbf{b})$ . However, if there is a centring vector which has components in both subspaces  $V(\mathbf{a}, \mathbf{b})$ ,  $V(\mathbf{c})$ , then the lattice  $T_G$  can be expressed as  $T(\mathbf{a}, \mathbf{b}) \oplus T(\mathbf{c})[\mathbf{0} + \mathbf{d}]$ .

*Definition 3.2.* Let  $(G, T_G)$  be an oriented arithmetic class with fixed parameters and let the action of  $G$  on  $V(n)$  be reducible (hence also decomposable), so that  $V(n) = V(k_1) \oplus V(k_2)$ . Further, let  $\sigma_1 : V(n) \rightarrow V(k_1)$  and  $\sigma_2 : V(n) \rightarrow V(k_2)$  be the projections of the space  $V(n)$  onto its  $G$ -invariant subspaces

**Table 1**

Reductions and decompositions of two-dimensional translation groups according to their Bravais classes.

Oblique system			
Any basis vectors $\mathbf{a}, \mathbf{b}$			
All reductions inclined		$T_{G1}^o$	$T_{G2}^o$
$p$	$T(\mathbf{a}) \oplus T(\mathbf{b})$	$\not\!/\!_a$	$\not\!/\!_b$
Rectangular system			
All reductions orthogonal			
$p$	$T(\mathbf{a}) \oplus T(\mathbf{b})$	$\not\!/\!_a$	$\not\!/\!_b$
$c$	$T(\mathbf{a}) \oplus T(\mathbf{b})[\mathbf{0} \cup (\mathbf{a} + \mathbf{b})/2]$	$\not\!/\!_{a/2}$	$\not\!/\!_{b/2}$

Meaning of symbols:  $p = T(\mathbf{a}, \mathbf{b})$ ,  $c = T[(\mathbf{a} + \mathbf{b})/2, (\mathbf{a} - \mathbf{b})/2]$ ,  $\not\!/\!_a = T(\mathbf{a})$ ,  $\not\!/\!_b = T(\mathbf{b})$ ;  $\not\!/\!_{a/2} = T(\mathbf{a}/2)$ ,  $\not\!/\!_{b/2} = T(\mathbf{b}/2)$ .

Groups of oblique and rectangular system in two dimensions are reducible and the space  $V(\mathbf{a}, \mathbf{b})$  splits into a direct sum  $V(\mathbf{a}, \mathbf{b}) = V(\mathbf{a}) \oplus V(\mathbf{b})$ , where the subspaces  $V(\mathbf{a})$ ,  $V(\mathbf{b})$  are orthogonal in the case of rectangular system, but can be inclined in the case of the oblique system. This table shows the reduction or decomposition of crystallographic lattices. We consider also lattices that contain continuous components. There are the following types of such lattices in two dimensions:

$\not\!/\!_a \not\!/\!_b = T_G(\mathbf{a}) \oplus V_G(\mathbf{b})$ , or  $\not\!/\!_a \not\!/\!_b = V_G(\mathbf{a}) \oplus T_G(\mathbf{b})$ , and  $V(\mathbf{a}, \mathbf{b})$ .

Lattices of  $\not\!/\!_a \not\!/\!_b$  and  $\not\!/\!_a \not\!/\!_b$  are invariant only under the action of point groups of oblique or rectangular systems. The lattice  $V(\mathbf{a}, \mathbf{b})$  represents the whole space and is therefore invariant under the group  $\mathcal{O}(2)$  and hence under any two-dimensional point group.

The same decompositions and reductions are applicable to lattices of layer groups with the space of missing translations  $V(\mathbf{c})$ . Oblique lattices correspond to the triclinic/oblique system and monoclinic/oblique system with the space of missing translations inclined and orthogonal, respectively. Rectangular lattices correspond to the monoclinic/rectangular and orthorhombic/rectangular and the space of missing translations is again inclined in the first and orthogonal in the second case. Lattices of  $\not\!/\!_a \not\!/\!_b$  and  $\not\!/\!_a \not\!/\!_b$  are invariant only under the action of point groups of triclinic, monoclinic and rectangular systems. The lattice  $V(\mathbf{a}, \mathbf{b})$  is invariant under all subgroups of the cylindrical group  $D_{\infty,z} = \infty_z/m_zmm$ .

$V(k_1)$  and  $V(k_2)$ , so that  $\sigma_1(\mathbf{x}) = \mathbf{x}_1$  and  $\sigma_2(\mathbf{x}) = \mathbf{x}_2$  are components of a vector  $\mathbf{x}$  in the subspaces  $V(k_1)$  and  $V(k_2)$  and hence  $\mathbf{x} = \mathbf{x}_1 + \mathbf{x}_2$ . We define translation groups  $T_{G1}^{(o)} = \sigma_1(T_G)$ ,  $T_{G2}^{(o)} = \sigma_2(T_G)$  and  $T_{G1} = T_G \cap V(k_1)$ ,  $T_{G2} = T_G \cap V(k_2)$ . The group  $T_G$  is then generally expressed as

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

where

$$T_{G1}^{(o)} = T_{G1}[\mathbf{0} \cup \mathbf{d}_{12} \cup \dots \cup \mathbf{d}_{1p}]$$

and

$$T_{G2}^{(o)} = T_{G1}[\mathbf{0} \cup \mathbf{d}_{22} \cup \dots \cup \mathbf{d}_{2p}].$$

Vectors  $\mathbf{d}_i$ ,  $i = 2, \dots, p$ , here are the centring vectors and  $\mathbf{d}_{1i} = \sigma_1(\mathbf{d}_i)$ ,  $\mathbf{d}_{2i} = \sigma_2(\mathbf{d}_i)$  are their projections on subspaces  $V(k_1)$ ,  $V(k_2)$ , respectively.

We say that the lattice  $T_G$  is decomposable under the action of  $G$  with respect to decomposition  $V(n) = V(k_1) \oplus V(k_2)$  if  $T_G = T_{G1} \oplus T_{G2}$ . In this case, we obtain that  $T_{G1} = T_{G1}^{(o)}$  and  $T_{G2} = T_{G2}^{(o)}$ .

We say that the lattice  $T_G$  is reducible/indecomposable under the action of  $G$  with respect to decomposition  $V(n) = V(k_1) \oplus V(k_2)$  if  $T_{G1} \oplus T_{G2} \subset T_G \subset T_{G1}^{(o)} \oplus T_{G2}^{(o)}$ .

Below we consider decompositions and reductions of translation subgroups which are reducible under the action of point groups in two- and three-dimensional cases. For crystallographic groups and hence for discrete lattices such

**Table 2**

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

Triclinic system				
Any basis vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$				
All reductions inclined			$T_{G1}^o$	$T_{G2}^o$
$P$	$T(\mathbf{a}, \mathbf{b}) \oplus T(\mathbf{c})$		$P_{ab}$	$\not\sim \ell_c$
Monoclinic system				
Orthogonal reduction, unique axis $\mathbf{c}$			$T_{G1}^o$	$T_{G2}^o$
$P$	$T(\mathbf{a}, \mathbf{b}) \oplus T(\mathbf{c})$		$P_{ab}$	$\not\sim \ell_c$
$A$	$T(\mathbf{a}, \mathbf{b}) \oplus T(\mathbf{c})[\mathbf{0} \cup (\mathbf{b} + \mathbf{c})/2]$		$P_{a,b/2}$	$\not\sim \ell_{c/2}$
$B$	$T(\mathbf{a}, \mathbf{b}) \oplus T(\mathbf{c})[\mathbf{0} \cup (\mathbf{a} + \mathbf{c})/2]$		$P_{a/2,b}$	$\not\sim \ell_{c/2}$
$I$	$T(\mathbf{a}, \mathbf{b}) \oplus T(\mathbf{c})[\mathbf{0} \cup (\mathbf{a} + \mathbf{b} + \mathbf{c})/2]$		$c_{ab}$	$\not\sim \ell_{c/2}$
Inclined reduction, unique axis $\mathbf{a}$			$T_{G1}^o$	$T_{G2}^o$
$P$	$T(\mathbf{a}, \mathbf{b}) \oplus T(\mathbf{c})$		$P_{ab}$	$\not\sim \ell_c$
$C$	$T[(\mathbf{a} + \mathbf{b})/2, (\mathbf{a} - \mathbf{b})/2] \oplus T(\mathbf{c})$		$c_{ab}$	$\not\sim \ell_c$
$B$	$T(\mathbf{a}, \mathbf{b}) \oplus T(\mathbf{c})[\mathbf{0} \cup (\mathbf{a} + \mathbf{c})/2]$		$P_{a/2,b}$	$\not\sim \ell_{c/2}$
$I$	$T(\mathbf{a}, \mathbf{b}) \oplus T(\mathbf{c})[\mathbf{0} \cup (\mathbf{a} + \mathbf{b} + \mathbf{c})/2]$		$c_{ab}$	$\not\sim \ell_{c/2}$
Inclined reduction, unique axis $\mathbf{b}$			$T_{G1}^o$	$T_{G2}^o$
$P$	$T(\mathbf{a}, \mathbf{b}) \oplus T(\mathbf{c})$		$P_{ab}$	$\not\sim \ell_c$
$C$	$T[(\mathbf{a} + \mathbf{b})/2, (\mathbf{a} - \mathbf{b})/2] \oplus T(\mathbf{c})$		$c_{ab}$	$\not\sim \ell_c$
$A$	$T(\mathbf{a}, \mathbf{b}) \oplus T(\mathbf{c})[\mathbf{0} \cup (\mathbf{b} + \mathbf{c})/2]$		$P_{a,b/2}$	$\not\sim \ell_{c/2}$
$I$	$T(\mathbf{a}, \mathbf{b}) \oplus T(\mathbf{c})[\mathbf{0} \cup (\mathbf{a} + \mathbf{b} + \mathbf{c})/2]$		$c_{ab}$	$\not\sim \ell_{c/2}$
Orthorhombic system				
All reductions orthogonal			$T_{G1}^o$	$T_{G2}^o$
$P$	$T(\mathbf{a}, \mathbf{b}) \oplus T(\mathbf{c})$		$P_{ab}$	$\not\sim \ell_c$
$C$	$T[(\mathbf{a} + \mathbf{b})/2, (\mathbf{a} - \mathbf{b})/2] \cup T(\mathbf{c})$		$c_{ab}$	$\not\sim \ell_c$
$B$	$T(\mathbf{a}, \mathbf{b}) \oplus T(\mathbf{c})[\mathbf{0} \cup (\mathbf{a} + \mathbf{c})/2]$		$P_{a/2,b}$	$\not\sim \ell_{c/2}$
$A$	$T(\mathbf{a}, \mathbf{b}) \oplus T(\mathbf{c})[\mathbf{0} \cup (\mathbf{b} + \mathbf{c})/2]$		$P_{a,b/2}$	$\not\sim \ell_{c/2}$
$F$	$T[(\mathbf{a} + \mathbf{b})/2, (\mathbf{a} - \mathbf{b})/2] \oplus T(\mathbf{c})[\mathbf{0} \cup (\mathbf{a} + \mathbf{c})/2]$		$P_{a/2,b/2}$	$\not\sim \ell_{c/2}$
$I$	$T(\mathbf{a}, \mathbf{b}) \oplus T(\mathbf{c})[\mathbf{0} \cup (\mathbf{a} + \mathbf{b} + \mathbf{c})/2]$		$c_{ab}$	$\not\sim \ell_{c/2}$
Tetragonal system				
All reductions orthogonal			$T_{G1}^o$	$T_{G2}^o$
$P$	$T(\mathbf{a}, \mathbf{b}) \cup T(\mathbf{c})$		$P_{ab}$	$\not\sim \ell_c$
$I$	$T(\mathbf{a}, \mathbf{b}) \oplus T(\mathbf{c})[\mathbf{0} \cup (\mathbf{a} + \mathbf{b} + \mathbf{c})/2]$		$\bar{P}_{ab}$	$\not\sim \ell_{c/2}$
Hexagonal family				
All reductions orthogonal				
Single $Z$ -decomposition ( $P$ ) only in hexagonal system				
Either $Z$ -decomposition ( $P$ ) or $Z$ -reduction ( $R$ ) in trigonal system.				
$P$	$T(\mathbf{a}, \mathbf{b}) \oplus T(\mathbf{c})$		$T_{G1}^o$	$T_{G2}^o$
$R_1$ (inverse setting)	$T(\mathbf{a}, \mathbf{b}) \oplus T(\mathbf{c})[\mathbf{0} \cup (2\mathbf{a} + \mathbf{b} + \mathbf{c})/3 \cup (\mathbf{a} + 2\mathbf{b} + 2\mathbf{c})/3]$		$\bar{P}_{ab}$	$\not\sim \ell_c$
$R_2$ (reverse setting)	$T(\mathbf{a}, \mathbf{b}) \oplus T(\mathbf{c})[\mathbf{0} \cup (\mathbf{a} + 2\mathbf{b} + \mathbf{c})/3 \cup (2\mathbf{a} + \mathbf{b} + 2\mathbf{c})/3]$		$\bar{P}_{1/3}$	$\not\sim \ell_{c/3}$

Meanings of symbols:  $p_{ab} = T(\mathbf{a}, \mathbf{b})$ ,  $p_{a/2,b} = T(\mathbf{a}/2, \mathbf{b})$ ,  $p_{a,b/2} = T(\mathbf{a}, \mathbf{b}/2)$ ,  $p_{a/2,b/2} = T(\mathbf{a}/2, \mathbf{b}/2)$ ;  $c_{ab} = T(\mathbf{a}) \oplus T[(\mathbf{a} + \mathbf{b})/2] = T[(\mathbf{a} + \mathbf{b})/2, (\mathbf{a} - \mathbf{b})/2]$  in the orthorhombic system;  $\hat{p}_{ab} = T(\mathbf{a}) \oplus T[(\mathbf{a} + \mathbf{b})/2] = T[(\mathbf{a} + \mathbf{b})/2, (\mathbf{a} - \mathbf{b})/2]$  in the tetragonal system;  $\bar{p}_{1/3} = T[(2\mathbf{a} + \mathbf{b})/3, (\mathbf{a} + 2\mathbf{b})/3]$ ,  $\not\sim \ell_c = T(\mathbf{c})$ ,  $\not\sim \ell_{c/2} = T(\mathbf{c}/2)$ ,  $\not\sim \ell_{c/3} = T(\mathbf{c}/3)$ .

The reductions and decompositions in this table are given with respect to decomposition of the whole vector space into a direct product  $V(\mathbf{a}, \mathbf{b}, \mathbf{c}) = V(\mathbf{a}, \mathbf{b}) \oplus V(\mathbf{c})$ . There exist also semicontinuous and continuous lattices that decompose under the action of certain point groups. We denote them as follows:  $p_{ab}v_c = T_G(\mathbf{a}, \mathbf{b}) \oplus V_G(\mathbf{c})$  or  $v_{ab}\not\sim \ell_c = V_G(\mathbf{a}, \mathbf{b}) \oplus T_G(\mathbf{c})$  and  $V(\mathbf{a}, \mathbf{b}, \mathbf{c})$ .

The first two lattices are invariant under all specific orientations of all point groups with the exception of cubic and icosahedral groups as well as under the special or full orthogonal groups  $\mathcal{SO}(3)$  and  $\mathcal{O}(3)$ . Quite generally, they are invariant under all subgroups of the cylindrical group  $D_{\infty,2} = \infty_2/m,mm$ .

The translation group  $V(\mathbf{a}, \mathbf{b}, \mathbf{c})$  represents the whole vector space and is therefore invariant under any of the three-dimensional point groups.

reductions and decompositions are given in Tables 1 and 2, respectively. Our consideration is, however, limited neither to space nor to crystallographic groups. General classification of Euclidean groups according to the character of their lattices follows below. Both tables are complemented with symbols for lattices of semicontinuous or continuous character in respective dimensions. Table 1 actually applies also to decompositions or reductions of lattices of layer groups.

*Classification by the character of the translation subgroup:* We shall consider only those groups, the lattices  $T_G$  of which contain only a discrete component  $T_d$  and/or continuous component  $V_c$ . Such a lattice is of the general form

$$T_G = T_d(\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_{k_d}) \oplus V_c(\mathbf{a}_{k_d+1}, \mathbf{a}_{k_d+2}, \dots, \mathbf{a}_{k_d+k_c})$$

and the whole vector space splits into a direct sum:

$$V(n) = V_d(k_d) \oplus V_c(k_c) \oplus V_l(d),$$

where  $V_d(k_d) = \langle T_d \rangle_R$  is the linear envelope of the discrete part and  $V_l(d)$  is the complement to the linear envelope  $\langle T_G \rangle_R$ , called here the *space of missing translations*. All three subspaces  $V_d(k_d)$ ,  $V_c(k_c)$  and  $V_l(d)$  must certainly be  $G$ -invariant. In general, we do not require that this complement be orthogonal to  $\langle T_G \rangle_R$  but we require it to be  $G$ -invariant.

*Definition 3.3.* We say that the lattice  $T_G$  is:

- (i) *continuous*, when  $k_d = 0$ ,  $k_c > 0$ ;
- (ii) *semicontinuous*, when  $k_d > 0$ ,  $k_c > 0$ ;



(iii) *discrete*, when  $k_d > 0$ ,  $k_c = 0$ .

For up to three-dimensional lattices, we then have the following lattice types:

$n - d = k_l = 1$ :  $\not\mu$  discrete,  $\nu$  continuous;

$n - d = k_l = 2$ :  $p, c$  discrete,  $\nu$  continuous,  $\not\mu\nu$  semicontinuous;

$n - d = k_l = 3$ :  $P, I, F, A \approx B \approx C, R$  discrete Bravais lattices,  $V$  continuous,  $p\nu, c\nu, \not\mu\nu$  semicontinuous.

Although this distinction of Euclidean groups according to the type of their lattices applies in arbitrary dimensions, up to three dimensions we have restrictions. Thus, in two dimensions, there are no frieze groups with a semicontinuous lattice, in three dimensions, only the combination of one-dimensional discrete and another one-dimensional continuous lattice is allowed for layer groups with semicontinuous lattices. The letters  $\nu, \nu$  and  $V$  have the meaning of vector spaces of dimensions one, two, and three. We use script lower-case fonts  $\not\mu$  and  $\nu$  for the discrete and continuous one-dimensional lattice in accordance with *ITE*. We suggest the use of the following names for groups with continuous and semicontinuous lattices:

point-like line, frieze and rod groups for groups with the lattice  $\nu$ ;

point-like plane and layer groups for groups with the lattice  $\nu$ ;

point-like space groups for groups with the lattice  $V$ ;

frieze-like plane groups and rod-like layer groups for the groups with the lattice  $\not\mu\nu$ .

layer-like space groups for groups with lattices  $p\nu$  or  $c\nu$ ;

rod-like space groups for groups with the lattice  $\not\mu\nu$ .

These names express certain properties of the groups. For example, in the case of a point-like space group  $VG$ , each point of the space has the same symmetry  $G$ . In the case of layer-like space groups, each plane with the orientation defined by the discrete part  $p$  or  $c$  of the lattice has the symmetry of the same layer group, while, in the case of rod-like space groups, each line with the orientation defined by the discrete part  $\not\mu$  of the lattice has the symmetry of the same rod group.

## 4. Amendments to classical terminology

### 4.1. Space, subperiodic and site-point groups

Consideration of new types of groups of three-dimensional space requires certain natural amendments to current terminology. Our first proposal is to amend the concept of space and subperiodic groups as follows.

#### ***The first amendment to standard terminology:***

**Definition 4.1.** The group  $\mathcal{G} = \{G, T_G, P, \mathbf{u}_G(g)\}$  is called:

(i) a *space group* if  $T_G$  spans the whole space  $V(n)$ ;

(ii) a *subperiodic group* if  $T_G$  spans a proper subspace  $V_l(k_l)$ ; the number  $d = n - k_l$  is called the *dimension deficiency* of the subperiodic group;

(iii) a *site-point group* if  $T_G = \{\mathbf{0}\}$ , so that it contains only the vector  $\mathbf{t} = \mathbf{0}$ ; we say also that  $T_G$  is trivial.

Up to four dimensions, we have the following, already adopted, nomenclature:

dimension 1:  $n = 1, d = 0$  line groups;

dimension 2:  $n = 2, d = 0$  plane groups;  $d = 1, k_l = 1$  frieze groups;

dimension 3:  $n = 3, d = 0$  space groups;  $d = 1, k_l = 2$  layer groups;  $d = 2, k_l = 1$  rod groups;

dimension 4:  $n = 4, d = 1, k_l = 3$  magnetic space groups (Shubnikov groups);  $d = 2, k_l = 2$  magnetic layer groups;  $d = 3, k_l = 1$  magnetic rod groups.

Note that we do not require here the discreteness of the lattice  $T_G$  so that the concept of space groups is extended to other than crystallographic groups. Below we also amend the concept of crystallographic groups. The term space group in non-traditional meaning is already in use for so-called quasi-crystallographic space groups and it is an adequate and natural terminology (Rokhsar *et al.*, 1988).

### 4.2. Crystallographic groups

#### ***The second amendment to standard terminology:***

**Definition 4.2a.** A point group  $G$  is called crystallographic if a discrete  $G$ -invariant  $T_G$  exists which spans the whole  $V(n)$ . [More mathematically:  $G$  affords  $Z$  representation on  $V(n)$  (Curtis & Reiner, 1966).]

**Definition 4.2b.** An Euclidean group  $\mathcal{G} = \{G, T_G, P, \mathbf{u}_G(g)\}$  is called crystallographic if its point group  $G$  is crystallographic.

#### *Justification of the changes to standard terminology.*

**Example:** The point-like space group  $Vm\bar{3}m$  is the symmetry of a crystal of point symmetry  $m\bar{3}m$  in the continuous approximation. The group certainly deserves the name space as well as crystallographic.

It is customary in the theory of phase transitions to handle the equitranslational cases in continuous approximation and in terms of point groups and tensor components. Even in this approximation, it is more rigorous to replace the point groups by point-like space groups and tensor components by tensor fields constant throughout the crystal. This is particularly evident in consideration of domain walls where the symmetry of the wall should be described by some layer group; in a rigorous use of the continuous approximation, we should use the point-like layer group.

The groups with continuous and semicontinuous lattices appear also as normalizers of space groups [*cf.* Koch & Fischer (1987); see also more detailed consideration of translation normalizer by Kopský (1993*bc*)]. Both amendments were proposed at ECM-9 in Prague in 1998 (Kopský, 2000).

### 5. Factorization of reducible three-dimensional space groups to layer and rod groups

In the following, we shall say that an Euclidean group  $\mathcal{G}$  is reducible if its translation subgroup  $T_G$  is reducible or decomposable under the action of the point group  $G$ . Reducibility (hence decomposability) of the point group  $G$  on  $V(n)$  is necessary and sufficient for either of these cases to appear. A quite general situation is considered by Kopský (1986), reducibility of three-dimensional space groups by Kopský (1988*b*, 1989*a,b*, 1993*a*) and Fuksa & Kopský (1993). The detailed theory is based on the application of the concept of *subdirect products* for reducible point groups and of *subdirect sums* for translation subgroups (see Kopský, 1988*a*). This concept actually also lies in the background of derivation of magnetic, black and white, symmetry–antisymmetry, colour groups and other generalizations. The fact that factorization of reducible or decomposable Euclidean groups leads to subperiodic groups is one of the most important consequences. Below we analyse the case of reducible three-dimensional space groups. In an analytical approach, we show that reducibility implies the existence of a layer and a rod group as factor groups of the space group. In a constructive approach, we show how a reducible space group can be assigned to a pair of layer and rod groups of the same reducible geometric class.

*Analytic approach:* Let  $\mathcal{G} = \{G, T_G, P, \mathbf{u}_G(g)\}$  be a reducible space group with decomposable action of  $G$  on  $T(\mathbf{a}, \mathbf{b}, \mathbf{c}) = T(\mathbf{a}, \mathbf{b}) \oplus T(\mathbf{c})$ , where  $T(\mathbf{a}, \mathbf{b}), T(\mathbf{c})$  are  $G$ -invariant. The system of non-primitive translations splits into its components  $\mathbf{u}_{G1}(g) \in V(\mathbf{a}, \mathbf{b})$  and  $\mathbf{u}_{G2}(g) \in V(\mathbf{c})$ , and  $\mathbf{u}_{G1}(g), \mathbf{u}_{G2}(g)$  satisfy Frobenius congruences mod  $T(\mathbf{a}, \mathbf{b})$  and mod  $T(\mathbf{c})$ , respectively. Hence, there exists a layer group  $\mathcal{L}$  and a rod group  $\mathcal{R}$ :

$$\mathcal{L} = \{G, T(\mathbf{a}, \mathbf{b}), P, \mathbf{u}_{G1}(g)\}, \quad \mathcal{R} = \{G, T(\mathbf{c}), P, \mathbf{u}_{G2}(g)\}.$$

The translation subgroups  $T(\mathbf{a}, \mathbf{b}), T(\mathbf{c})$  are normal in  $\mathcal{G}$  and the factor groups are isomorphic to this layer and rod group:

$$\mathcal{L} \approx \mathcal{G}/T(\mathbf{c}) \quad \text{and} \quad \mathcal{R} \approx \mathcal{G}/T(\mathbf{a}, \mathbf{b}).$$

*This result is of particular importance in the representation theory of space groups and in the theory of the lattices of their subgroups.*

Indeed, it follows that representations of the layer group  $\mathcal{L}$  and of the rod group  $\mathcal{R}$  engender certain representations of the space group  $\mathcal{G}$  and that the lattices of subgroups of the layer and rod groups are isomorphic with certain sublattices of the space group (Kopský, detailed consideration will be published).

*Constructive approach:* We take all layer and rod groups of arithmetic classes  $(G, T(\mathbf{a}, \mathbf{b}))$  and  $(G, T(\mathbf{c}))$ :

$$\mathcal{L}^{(\omega)}(\mu) = \{G, T(\mathbf{a}, \mathbf{b}), P, \mathbf{u}_{G1}^{(\omega)}(g) + \varphi(g, \mu)\},$$

$$\mathcal{R}^{(\beta)}(v) = \{G, T(\mathbf{c}), P, \mathbf{u}_{G2}^{(\beta)}(g) + \varphi(g, v)\}$$

and by their combination we get all space groups of the arithmetic class  $(G, T(\mathbf{a}, \mathbf{b}, \mathbf{c}))$ :

$$\mathcal{G}^{(\alpha, \beta)}(\mu + v) = \{G, T(\mathbf{a}, \mathbf{b}, \mathbf{c}), P, \mathbf{u}_G^{(\alpha, \beta)}(g) + \varphi(g, \mu + v)\}.$$

#### 5.1. Schreier multiplication

It is therefore possible to introduce a formal multiplication of the symbols of complementary subperiodic groups where the result is a space group:

$$\mathcal{G}^{(\alpha, \beta)}(\mu + v) = \mathcal{L}^{(\alpha)}(\mu) \diamond \mathcal{R}^{(\beta)}(v),$$

which corresponds to

$$T(\mathbf{a}, \mathbf{b}, \mathbf{c}) = T(\mathbf{a}, \mathbf{b}) \oplus T(\mathbf{c}), \quad \mathbf{u}_G^{(\alpha, \beta)}(g) = \mathbf{u}_{G1}^{(\alpha)}(g) + \mathbf{u}_{G2}^{(\beta)}(g),$$

$$\varphi(g, \mu + v) = \varphi(g, \mu) + \varphi(g, v).$$

We name this law after Schreier (1926*a,b*), the initiator of the theory of group extensions.

*This result and Theorem 2 create the background for the ‘Unified system of Hermann–Mauguin symbols’ for space and subperiodic groups.*

*Remark 4.* If either of the components  $T(\mathbf{a}, \mathbf{b})$  or  $T(\mathbf{c})$  is replaced by continuous translation subgroup  $V(\mathbf{a}, \mathbf{b})$  or  $V(\mathbf{c})$ , then there exists only one respective system of non-primitive translations which is trivial.

All three-dimensional point groups with the exception of cubic groups are reducible and their action on lattices of primitive Bravais type  $P$  is decomposable. Centred lattices are generally only reducible and, although the factorization theorem also holds for them, it has a slightly different form which will be considered in detail in another paper. However, the decomposition used above applies for the centring in the  $(\mathbf{a}, \mathbf{b})$  plane and the resulting layer groups have then a centred lattice. This happens in cases of monoclinic and orthorhombic lattices when  $C$ -centring of a space group implies  $c$ -centring of layer groups, which are the results of factorization. Decompositions  $T(\mathbf{a}, \mathbf{b}, \mathbf{c}) = T(\mathbf{a}) \oplus T(\mathbf{b}, \mathbf{c})$  and  $T(\mathbf{a}, \mathbf{b}, \mathbf{c}) = T(\mathbf{b}) \oplus T(\mathbf{a}, \mathbf{c})$  also lead to factorization and can be applied for  $A$ - and  $B$ -centring.

The primitive lattices of layer groups in cases of triclinic, monoclinic and orthorhombic groups are themselves decomposable. Corresponding factor groups are then the rod groups of the same geometric class. Quite generally, if the lattice of a space group  $\mathcal{G}$  of arithmetic class  $(G, T_G)$  decomposes into the direct sum  $T_G = T(\mathbf{a}, \mathbf{b}, \mathbf{c}) = T(\mathbf{a}) \oplus T(\mathbf{b}) \oplus T(\mathbf{c})$ , then the systems of non-primitive translations (SNTs) of this space group splits into a sum  $\mathbf{u}_G(g) = \mathbf{u}_G^{(\alpha, \beta, \gamma)}(g) = \mathbf{u}_{Ga}^{(\alpha)}(g) + \mathbf{u}_{Gb}^{(\beta)}(g) + \mathbf{u}_{Gc}^{(\gamma)}(g)$ , where  $\mathbf{u}_{Ga}^{(\alpha)}(g) \in V(\mathbf{a}), \mathbf{u}_{Gb}^{(\beta)}(g) \in V(\mathbf{b}), \mathbf{u}_{Gc}^{(\gamma)}(g) \in V(\mathbf{c})$ , each of which satisfies Frobenius congruences  $\mathbf{w}_a^{(\alpha)}(g, h) \in T(\mathbf{a}), \mathbf{w}_b^{(\beta)}(g, h) \in T(\mathbf{b}), \mathbf{w}_c^{(\gamma)}(g, h) \in T(\mathbf{c})$  so that they define rod groups  $\mathcal{R}_a^{(\alpha)}, \mathcal{R}_b^{(\beta)}$  and  $\mathcal{R}_c^{(\gamma)}$ .

The shift function  $\varphi(g, \mathbf{s})$  also splits into its components  $\varphi_a(g, \mu), \varphi_b(g, v), \varphi_c(g, \tau)$  in spaces  $V(\mathbf{a}), V(\mathbf{b}), V(\mathbf{c})$ , where  $\mathbf{s} = \mu + v + \tau, \mu \in V(\mathbf{a}), v \in V(\mathbf{b}), \tau \in V(\mathbf{c})$ , and any space group of the oriented arithmetic class  $(G, T_G)$  with fixed parameters can be expressed as

**Table 3**

Systems of non-primitive translations for rod, layer and space groups of geometric classes  $C_{4h} - 4/m$  and  $C_{4v} - 4mm$ .

(a) Geometric class  $C_{4h} - 4/m$

Arithmetic classes:		$4/m\bar{h}$	$4/mp$	$4/mP$		
Cohomology groups:		$C_2 = C(\alpha_2)$	$C_2 = C(\alpha_1)$	$C_2^3 = C(\alpha_1, \alpha_2)$		
Cohomology element	Arithmetic class	Group type	$4_z$	$2_z$	$4_z^{-1}$	$i$
$\varepsilon_2$	$4/m\bar{h}$	$\bar{h}4/m$	<b>0</b>	<b>0</b>	<b>0</b>	<b>0</b>
$\alpha_2$	Rod	$\bar{h}4_2/m$	<b>c/2</b>	<b>0</b>	<b>c/2</b>	<b>0</b>
$\varepsilon_1$	$4/mp$	$p4/m$	<b>0</b>	<b>0</b>	<b>0</b>	<b>0</b>
$\alpha_1$	Layer	$p4/n$	<b>0</b>	<b>0</b>	<b>0</b>	<b>(a + b)/2</b>
$\varepsilon_1$	$4/mP$	$P4/m$	<b>0</b>	<b>0</b>	<b>0</b>	<b>0</b>
$\alpha_2$	Space	$P4_2/m$	<b>c/2</b>	<b>0</b>	<b>c/2</b>	<b>0</b>
$\alpha_1$		$P4/n$	<b>0</b>	<b>0</b>	<b>0</b>	<b>(a + b)/2</b>
$\alpha_1\alpha_2$		$P4_2/n$	<b>c/2</b>	<b>0</b>	<b>c/2</b>	<b>(a + b)/2</b>

  

$4_z$	$m_z$	$4_z^{-1}$	Correlation with space groups according to ITA		
<b>0</b>	<b>0</b>	<b>0</b>			
<b>c/2</b>	<b>0</b>	<b>c/2</b>			
<b>0</b>	<b>0</b>	<b>0</b>			
<b>(a + b)/2</b>	<b>(a + b)/2</b>	<b>(a + b)/2</b>		1	2
<b>0</b>	<b>0</b>	<b>0</b>	$C_{4h}^1$	<b>0</b>	–
<b>c/2</b>	<b>0</b>	<b>c/2</b>	$C_{4h}^2$	<b>0</b>	–
<b>(a + b)/2</b>	<b>(a + b)/2</b>	<b>(a + b)/2</b>	$C_{4h}^3$	<b>a/2</b>	<b>(a + b)/4</b>
<b>(a + b + c)/2</b>	<b>(a + b)/2</b>	<b>(a + b + c)/2</b>	$C_{4h}^4$	<b>a/2 + c/4</b>	<b>(a + 3b)/4</b>

(b) Geometric class  $C_{4v} - 4mm$

Arithmetic classes:		$4mm\bar{h}$	$4mmp$	$4mmP$	
Cohomology groups:		$C_2^3 = C(\alpha_2, \beta_2)$	$C_2 = C(\alpha_1)$	$C_2^3 = C(\alpha_1, \alpha_2, \beta_2)$	
Cohomology element	Arithmetic class	Group type	$4_z$	$2_z$	$4_z^{-1}$
$\varepsilon_2$	$4mm\bar{h}$	$\bar{h}4mm$	<b>0</b>	<b>0</b>	<b>0</b>
$\alpha_2$	Rod	$\bar{h}4_2cm$	<b>c/2</b>	<b>0</b>	<b>c/2</b>
$\beta_2$		$\bar{h}4_2mc$	<b>c/2</b>	<b>0</b>	<b>c/2</b>
$\alpha_2\beta_2$		$\bar{h}4cc$	<b>0</b>	<b>0</b>	<b>0</b>
$\varepsilon_1$	$4mmp$	$p4mm$	<b>0</b>	<b>0</b>	<b>0</b>
$\alpha_1$	Layer	$p4bm$	<b>0</b>	<b>0</b>	<b>0</b>
$\varepsilon$	$4mmP$	$P4mm$	<b>0</b>	<b>0</b>	<b>0</b>
$\alpha_1$	Space	$P4bm$	<b>0</b>	<b>0</b>	<b>0</b>
$\alpha_2$		$P4_2cm$	<b>c/2</b>	<b>0</b>	<b>c/2</b>
$\alpha_1\alpha_2$		$P4_2nm$	<b>c/2</b>	<b>0</b>	<b>c/2</b>
$\alpha_2\beta_2$		$P4cc$	<b>0</b>	<b>0</b>	<b>0</b>
$\alpha_1\alpha_2\beta_2$		$P4nc$	<b>0</b>	<b>0</b>	<b>0</b>
$\beta_2$		$P4_2mc$	<b>c/2</b>	<b>0</b>	<b>c/2</b>
$\alpha_1\beta_2$		$P4_2bc$	<b>c/2</b>	<b>0</b>	<b>c/2</b>

  

$m_x$	$m_{xy}$	$m_y$	$m_{xy}$	Correlation with space groups according to ITA	
<b>0</b>	<b>0</b>	<b>0</b>	<b>0</b>		
<b>c/2</b>	<b>0</b>	<b>c/2</b>	<b>0</b>		
<b>0</b>	<b>c/2</b>	<b>0</b>	<b>c/2</b>		
<b>c/2</b>	<b>c/2</b>	<b>c/2</b>	<b>c/2</b>		
<b>0</b>	<b>0</b>	<b>0</b>	<b>0</b>		
<b>(a + b)/2</b>	<b>(a + b)/2</b>	<b>(a + b)/2</b>	<b>(a + b)/2</b>		
<b>0</b>	<b>0</b>	<b>0</b>	<b>0</b>	$C_{4v}^1$	<b>0</b>
<b>(a + b)/2</b>	<b>(a + b)/2</b>	<b>(a + b)/2</b>	<b>(a + b)/2</b>	$C_{4v}^2$	<b>0</b>
<b>c/2</b>	<b>0</b>	<b>c/2</b>	<b>0</b>	$C_{4v}^3$	<b>0</b>
<b>(a + b + c)/2</b>	<b>(a + b)/2</b>	<b>(a + b + c)/2</b>	<b>(a + b)/2</b>	$C_{4v}^4$	<b>a/2</b>
<b>c/2</b>	<b>c/2</b>	<b>c/2</b>	<b>c/2</b>	$C_{4v}^5$	<b>0</b>
<b>(a + b + c)/2</b>	<b>(a + b + c)/2</b>	<b>(a + b + c)/2</b>	<b>(a + b + c)/2</b>	$C_{4v}^6$	<b>0</b>
<b>0</b>	<b>c/2</b>	<b>0</b>	<b>c/2</b>	$C_{4v}^7$	<b>0</b>
<b>(a + b)/2</b>	<b>(a + b + c)/2</b>	<b>(a + b)/2</b>	<b>(a + b + c)/2</b>	$C_{4v}^8$	<b>0</b>

$$\mathcal{G}^{(\alpha,\beta,\gamma)}(\mathbf{s}) = \mathcal{R}_a^{(\alpha)}(\mu) \diamond \mathcal{R}_b^{(\beta)}(\nu) \diamond \mathcal{R}_c^{(\gamma)}(\tau).$$

There also exist layer groups

$$\begin{aligned} \mathcal{L}_{ab}^{(\alpha,\beta)}(\mu + \nu) &= \mathcal{R}_a^{(\alpha)}(\mu) \diamond \mathcal{R}_b^{(\beta)}(\nu), \\ \mathcal{L}_{bc}^{(\beta,\gamma)}(\nu + \tau) &= \mathcal{R}_b^{(\beta)}(\nu) \diamond \mathcal{R}_c^{(\gamma)}(\tau), \\ \mathcal{L}_{ca}^{(\gamma,\alpha)}(\tau + \mu) &= \mathcal{R}_c^{(\gamma)}(\tau) \diamond \mathcal{R}_a^{(\alpha)}(\mu) \end{aligned}$$

and the space groups can also be expressed as

$$\begin{aligned} \mathcal{G}^{(\alpha,\beta,\gamma)}(\mathbf{s}) &= \mathcal{L}_{ab}^{(\alpha,\beta)}(\mu + \nu) \diamond \mathcal{R}_c^{(\gamma)}(\tau) \\ &= \mathcal{L}_{bc}^{(\beta,\gamma)}(\nu + \tau) \diamond \mathcal{R}_a^{(\alpha)}(\mu) \\ &= \mathcal{L}_{ca}^{(\gamma,\alpha)}(\tau + \mu) \diamond \mathcal{R}_b^{(\beta)}(\nu). \end{aligned}$$

There are three ways to illustrate the relationship between decomposable space groups and respective layer and rod groups (decomposable plane and frieze groups or decomposable layer and rod groups).

(i) By tables of systems of non-primitive translations; two examples are given in Table 3.

(ii) By tables of Hermann–Mauguin symbols; here we can observe either how the symbol of the space group splits into a pair of symbols for layer and rod group or how these two combine into the symbol of the space group (frieze groups into plane groups or rod groups into layer groups). This will be illustrated in §7.

(iii) By comparison of group diagrams.

SNTs for rod, layer and space groups of geometric classes  $C_{4h} - 4/m$  and  $C_{4v} - 4mm$  are given in Table 3. The space groups in Tables 3(a) and 3(b) belong to arithmetic classes with primitive lattice  $P$ , i.e. to  $4/mP$  and  $4mmP$ , where the lattice decomposes into the direct sum  $P = \not\mu \oplus p$  and the rod groups therefore belong to arithmetic classes  $4/m\not\mu$  and  $4mm\not\mu$  and the layer groups to arithmetic classes  $4/mp$  and  $4mmp$ . For rod and layer groups, the SNTs correspond to standards given in *ITE*. For space groups they are chosen as the sums of SNTs of corresponding rod and layer groups.

From diagrams of space groups in *ITA*, we can deduce the SNTs that correspond to each diagram. However, the resulting SNTs do not always coincide with those we obtain from combination of SNTs of respective rod and layer groups. In the last column of Tables 3(a) and 3(b), we show the shifts that correspond to the different choices.

It is important to realize that SNTs do not always correspond to space- (or generally Euclidean) group types. Indeed, the SNT uniquely defines the diagram of the group. The label of the SNT ( $\alpha$  etc.) defines the diagram up to its shift in space. Hence, in the case of orthorhombic groups, where different diagrams correspond to different settings (orientation of the group with reference to crystallographic basis), there are several different diagrams to one space-group type. Each diagram corresponds to a certain label of SNT as well as to a quite specific Hermann–Mauguin symbol.

We know of only one source where SNTs are used. This is the book on crystallographic groups of four-dimensional space by Brown *et al.* (1978). Not all SNTs are presented in this book; in tables one can observe that the order of the co-

homology group is sometimes different from that of the space-group types. This is exactly the case of orthorhombic groups where the number of non-equivalent SNTs and hence the number of distinct diagrams for arithmetic class  $mmmP$  is 64 while the number of space-group types is 16.

The correspondence between SNTs and diagrams or Hermann–Mauguin symbols is incomplete in *ITA* in the case of space-group type  $T_h^6$  for which Hermann–Mauguin symbol  $Pa\bar{3}$  is used. If we rotate the diagram by  $90^\circ$ , we find that it is impossible to make the resulting picture coincide with the original. In crystallographic language, this means that this group has another setting and it should be indicated by the symbol  $Pb\bar{3}$  on the side of the diagrams. In the language of SNTs, this means that no shift function exists which will change the SNT for the symbol  $Pa\bar{3}$  to the SNT for the symbol  $Pb\bar{3}$ . The SNT for this group will be missing and the SNTs for groups  $T_h^1 - Pm\bar{3}$ ,  $T_h^6 - Pa\bar{3}$  and  $T_h^2 - Pn\bar{3}$  do not constitute a group.

*Comment:* The author must say with regret that no discussion with crystallographers helped him to understand what exact meaning they assign to Hermann–Mauguin symbols. It would be a waste of ingenious symbols to interpret them as symbols of space-group types – Schoenflies symbols are quite sufficient for that purpose.

## 6. Euclidean groups of reducible geometric classes

In this and the next section, we shall consider Euclidean groups of reducible geometric classes with reference to a certain reduction of the space with which decomposition of their lattices is associated. To each such case, we assign a certain chart which shows how these groups are related. These charts have a common structure as described below.

*Plane groups:* We assume that the space  $V(\mathbf{a}, \mathbf{b})$  splits under the action of the point group  $G$  into a direct sum  $V(\mathbf{a}) \oplus V(\mathbf{b})$ . The following lattices define the arithmetic classes:  $T(\mathbf{a}) \sim \not\mu_a$ ,  $V(\mathbf{a}) \sim v_a$ ,  $T(\mathbf{b}) \sim \not\mu_b$ ,  $V(\mathbf{b}) \sim v_b$ ,  $T(\mathbf{a}, \mathbf{b}) = T(\mathbf{a}) \oplus T(\mathbf{b}) \sim p$ ,  $V(\mathbf{a}) \oplus V(\mathbf{b}) \sim v_a v_b$ ,  $T(\mathbf{a}) \oplus V(\mathbf{b}) \sim \not\mu_a v_b$  and  $V(\mathbf{a}, \mathbf{b}) \sim v$ . Groups of the geometric class are arranged in blocks as shown in Table 4 with names of groups in each block.

*Layer groups:* The lattices are defined in the same way as for the plane groups. Instead of frieze (frieze-like) groups there are rod (and rod-like) groups and instead of plane groups there are layer groups. See Table 5.

*Space groups:* We assume that the space  $V(\mathbf{a}, \mathbf{b}, \mathbf{c})$  splits into a direct sum  $V(\mathbf{a}, \mathbf{b}) \oplus V(\mathbf{c})$ . The following lattices define the arithmetic classes:  $T(\mathbf{a}, \mathbf{b}) \sim p_{ab}$ ,  $V(\mathbf{a}, \mathbf{b}) \sim v_{ab}$ ,  $T(\mathbf{c}) \sim \not\mu_c$ ,  $V(\mathbf{c}) \sim v_c$ ,  $T(\mathbf{a}, \mathbf{b}, \mathbf{c}) = T(\mathbf{a}, \mathbf{b}) \oplus T(\mathbf{c}) \sim P$ ,  $V(\mathbf{a}, \mathbf{b}) \oplus V(\mathbf{c}) \sim v_{ab} v_c$ ,  $T(\mathbf{a}, \mathbf{b}) \oplus V(\mathbf{c}) \sim p_{ab} v_c$  and  $V(\mathbf{a}, \mathbf{b}, \mathbf{c}) \sim V$ . In cases of monoclinic and orthorhombic groups, there appears a subchart corresponding to arithmetic class  $GC$  of space groups with a  $C$ -centred lattice. In this case, the following lattices also appear:



**Table 4**  
Plane groups: primitive type/decomposition.

Arithmetic class	Frieze groups with discrete lattice	Frieze groups with continuous lattice
Frieze groups with discrete lattice	Reducible plane groups with primitive lattice	Frieze-like plane groups with semicontinuous lattice
Frieze group with continuous lattice	Frieze-like plane groups with semicontinuous lattice	Point-like plane groups with continuous lattice
$v_a$	$v_a/v_b$	$v$

**Table 5**  
Layer groups: primitive type/decomposition.

Arithmetic class	Rod groups with discrete lattice	Rod groups with continuous lattice
Rod groups with discrete lattice	Reducible layer groups with primitive lattice	Rod-like layer groups with semicontinuous lattice
Rod group with continuous lattice	Rod-like layer groups with semicontinuous lattice	Point-like layer groups with continuous lattice
$v_a$	$v_a/v_b$	$v$

**Table 6**  
Space groups: primitive type and decomposable cases.

Arithmetic class	Rod groups with discrete lattice	Rod groups with continuous lattice
Layer groups with discrete primitive lattice	Reducible space groups with primitive lattice	Space groups with semicontinuous lattice
Layer groups with discrete centred lattice	Reducible space groups with base-centred lattice in <i>C</i> setting	Layer-like space groups with semicontinuous lattice
Layer group with continuous lattice	Rod-like space groups with semicontinuous lattice	Point-like space groups with continuous lattice
$v_{ab}$	$v_{ab}/v_c$	$V$

$$T[(\mathbf{a} + \mathbf{b})/2, (\mathbf{a} - \mathbf{b})/2] \sim c_{ab},$$

$$T[(\mathbf{a} + \mathbf{b})/2, (\mathbf{a} - \mathbf{b})/2] \oplus T(\mathbf{c}) \sim C,$$

$$T[(\mathbf{a} + \mathbf{b})/2, (\mathbf{a} - \mathbf{b})/2] \oplus V(\mathbf{c}) \sim c_{ab}/v_c.$$

In actual charts, we refer to the decomposition and leave out the subscripts indicating subspaces.

All three charts (Tables 4, 5, 6) have the following common features. (i) In the left upper corner is given the arithmetic class of groups which appear in the central block. (ii) Each block contains groups of the same arithmetic class; the lattice and name of the kind of groups is given. (iii) The first column and the first row contain first the groups with discrete lattice, the last group in the row and column is the point-like group. (iv) On intersection of rows and columns, we find those groups that are obtained from groups heading the rows and columns. The lattice of these groups is the direct sum of the lattices and the SNTs are the sums of SNTs of groups heading the row and

column. As a result, the groups with semicontinuous lattices are arranged in the last row and column and the point-like group of the geometric class stands in the right lower corner. (v) A space shift of the group on the intersection is the sum of the space shifts of the groups heading the row and column.

### 7. Examples of charts of Euclidean groups with respect to the same decomposition of the space under the action of a reducible point group

The first three charts correspond to the point group  $C_{2v}$ . In the first chart (Table 7), we consider plane groups of this class as combinations of frieze groups. In the second chart (Table 8), we consider layer groups as combinations of rod groups. In both tables, we assume that the translation subgroups are generated by vectors **a** and **b**. Layer groups in Table 8 are usually called the ‘trivial’ layer groups and sometimes identified with plane groups because they do not contain an operation which exchanges the sides of the plane while the ‘true’ layer groups which do change the sides of the plane were called ‘groups of two-sided plane’ by Holser (1958*a,b*). This name is rather inappropriate because all planes in three-dimensional space have two sides. We interpret the plane groups as groups acting on two-dimensional space, which is to say a ‘plane in itself’, which has no sides, in contrast to planes in three-dimensional space, which are two-sided anyway and, in addition, they have a certain location in a direction complementary to the plane.

This is the reason why we preferred in *ITE* the symbols of layer groups by Bohm & Dornberger-Schiff (1966) to those used by Wood (1964). The latter were derived by the method of halving subgroups from plane groups in which, unfortunately, if we interpret them as groups in three-dimensional space, the first position of the symbol for oblique and rectangular systems corresponds to the direction perpendicular to the plane, while in corresponding symbols of monoclinic and orthorhombic systems this direction defines the last position of the Hermann–Mauguin symbol. Accordingly, the geometric class of plane groups is denoted by Hermann–Mauguin symbol  $2mm$  while the geometric class of (though trivial) layer groups is  $mm2$ . There exist, of course, also geometric classes of the type  $C_{2v}$  of other orientations to which there correspond Hermann–Mauguin symbols  $2mm$  and  $m2m$ .

The chart in Table 9 shows how the space groups of the same geometric class  $C_{2v} - mm2$  combine from layer and rod groups. We can see that the correspondence of symbols will never be achieved if we adopted Wood’s symbols for layer groups. In this chart, we also show how space groups with a *C*-centred lattice combine from layer groups with a *c*-centred lattice with rod groups. Layer groups from Table 8 are used here and the rod groups are of different types from those in Table 8 because the direction of the twofold axis coincides now with the translation space while in the previous case it is perpendicular to it.

In the chart in Table 10, we show how the groups of tetragonal classes  $422$ ,  $4mm$ ,  $42m$ ,  $4m2$  and  $4/mmm$  combine

**Table 7**

Plane groups of the geometric class  $C_{2v} - 2mm$ .

$2mm$	$\rho_b 2mm$	$\rho_b 2gm$	$v_b 2mm$
$\rho_a 2mm$	$p2mm$	$p2gm$	$\rho_a v_b 2mm$
$\rho_a 2mg$	$p2mg$	$p2gg$	$\rho_a v_b 2mg$
$v_a 2mm$	$v_a \rho_b 2mm$	$v_a \rho_b 2gm$	$v2mm$

**Table 8**

Layer groups of the geometric class  $C_{2v} - mm2$ .

$mm2p$	$\rho_b mm2$	$\rho_b bm2$	$v_b mm2$
$\rho_a mm2$	$pmm2$	$pbm2$	$\rho_a v_b mm2$
$\rho_a ma2$	$pma2$	$pba2$	$\rho_a v_b ma2$
$v_a mm2$	$v_a \rho_b mm2$	$v_a \rho_b bm2$	$vmm2$

**Table 9**

Space groups of the geometric class  $C_{2v} - mm2$ ; arithmetic classes  $mm2P$  and  $mm2C$ .

$mm2P$	$\rho mm2$	$\rho mc2_1$	$\rho cm2_1$	$\rho cc2$	$vmm2$
$pmm2$	<sup>1</sup> $Pmm2$	<sup>2</sup> $Pmc2_1$	<sup>2</sup> $Pcm2_1$	<sup>3</sup> $Pcc2$	$p\ vmm2$
$pma2$	<sup>4</sup> $Pma2$	<sup>7</sup> $Pmn2_1$	<sup>5</sup> $Pca2_1$	<sup>6</sup> $Pcn2$	$p\ vma2$
$pbm2$	<sup>4</sup> $Pbm2$	<sup>5</sup> $Pbc2_1$	<sup>7</sup> $Pnm2_1$	<sup>6</sup> $Pnc2$	$p\ vbm2$
$pba2$	<sup>8</sup> $Pba2$	<sup>9</sup> $Pbn2_1$	<sup>9</sup> $Pna2_1$	<sup>10</sup> $Pnn2$	$p\ vba2$
$mm2C$					
$cmm2$	<sup>11</sup> $Cmm2$	<sup>12</sup> $Cmc2_1$	<sup>12</sup> $Ccm2_1$	<sup>13</sup> $Ccc2$	$c\ vmm2$
$vmm2$	$v\ \rho mm2$	$v\ \rho mc2_1$	$v\ \rho cm2_1$	$v\ \rho cc2$	$Vmm2$

from corresponding layer and rod groups. Tables 9 and 10 illustrate simple rules on which the unification is based. Lattices on intersections are direct sums of lattices of layer and rod groups. On each position of a Hermann–Mauguin symbol, we combine the symbol in the rod group with that in the layer group according to known rules. Thus the screw axes  $4_1, 4_2, 4_3$  in rod groups combine with ordinary axis 4 in layer groups (where screws in this direction cannot exist) into  $4_1, 4_2, 4_3$  screw axes in the space group. Screw axes  $2_1$  of layer groups in the second or third position combine with ordinary axes 2 of rod groups (where screw axes in these directions cannot exist) into  $2_1$  screw axes of space groups. Only glide planes with symbol  $c$  are allowed in symbols of rod groups, while only  $a, b$  and  $n$  are allowed in symbols of layer groups. They combine among themselves and with the symbols  $m$  of ordinary planes as follows:  $(m, m) \approx m, (m, c) \approx c, (a, m) \approx a, (a, c) \approx n, (b, m) \approx b, (b, c) \approx n, (n, m) \approx n$ , while other combinations do not exist.

The Hermann–Mauguin symbols of the ordinary space groups are arranged in the central part of each table. The superscripts on the left are the numerical labels of the respective Schoenflies symbols of the space-group type. The first row contains symbols of rod groups of the arithmetic class  $G\rho$  which correspond to systems of non-primitive translations  $\mathbf{u}^{(\beta)}$ ; the first symbol  $\rho G$  is the symbol of the symmorphic rod group, the last symbol  $vG$  is the symbol of the point-like rod group – it is  $\mathbf{u}^{(\beta)} \equiv \mathbf{0}$  in both cases. The first column contains symbols of layer groups of the arithmetic class  $Gp$  which correspond to systems of non-primitive translations  $\mathbf{u}^{(\alpha)}$ ; the first symbol  $pG$  is the symbol of the symmorphic layer group,

**Table 10**

Correlation of Hermann–Mauguin symbols for space groups with those of layer and rod groups of tetragonal decomposable point groups.

Geometric class 422

$422P$	$\rho 422$	$\rho 4_1 22$	$\rho 4_2 22$	$\rho 4_3 22$	$v 422$
$p422$	<sup>1</sup> $P422$	<sup>3</sup> $P4_1 22$	<sup>5</sup> $P4_2 22$	<sup>7</sup> $P4_3 22$	$p\ v 422$
$p42_1 2$	<sup>2</sup> $P42_1 2$	<sup>4</sup> $P4_1 2_1 2$	<sup>6</sup> $P4_2 2_1 2$	<sup>8</sup> $P4_3 2_1 2$	$p\ v 42_1 2$
$v422$	$v\ \rho 422$	$v\ \rho 4_1 22$	$v\ \rho 4_2 22$	$v\ \rho 4_3 22$	$V 422$

Geometric class 4mm

$4mmP$	$\rho 4mm$	$\rho 4_2 cm$	$\rho 4cc$	$\rho 4_2 mc$	$v 4mm$
$p4mm$	<sup>1</sup> $P4mm$	<sup>3</sup> $P4_2 cm$	<sup>5</sup> $P4cc$	<sup>7</sup> $P4_2 mc$	$p\ v 4mm$
$p4bm$	<sup>2</sup> $P4bm$	<sup>4</sup> $P4_2 nm$	<sup>6</sup> $P4nc$	<sup>8</sup> $P4_2 bc$	$p\ v 4bm$
$v4mm$	$v\ \rho 4mm$	$v\ \rho 4_2 cm$	$v\ \rho 4cc$	$v\ \rho 4_2 mc$	$V 4mm$

Geometric class  $\bar{4}2m$

$\bar{4}2mP$	$\rho \bar{4}2m$	$\rho \bar{4}2c$	$v \bar{4}2m$
$p\bar{4}2m$	<sup>1</sup> $P\bar{4}2m$	<sup>2</sup> $P\bar{4}2c$	$p\ v \bar{4}2m$
$p\bar{4}2_1 m$	<sup>3</sup> $P\bar{4}2_1 m$	<sup>4</sup> $P\bar{4}2_1 c$	$p\ v \bar{4}2_1 m$
$v\bar{4}2m$	$v\ \rho \bar{4}2m$	$v\ \rho \bar{4}2c$	$V \bar{4}2m$

Geometric class  $\bar{4}m2$

$\bar{4}m2P$	$\rho \bar{4}m2$	$\rho \bar{4}c2$	$v \bar{4}m2$
$p\bar{4}m2$	<sup>5</sup> $P\bar{4}m2$	<sup>6</sup> $P\bar{4}c2$	$p\ v \bar{4}m2$
$p\bar{4}b2$	<sup>7</sup> $P\bar{4}b2$	<sup>8</sup> $P\bar{4}n2$	$p\ v \bar{4}b2$
$v\bar{4}m2$	$v\ \rho \bar{4}m2$	$v\ \rho \bar{4}c2$	$V \bar{4}m2$

Geometric class 4/mmmP

$4/mmmP$	$\rho 4/mmm$	$\rho 4/mcc$	$\rho 4_2/mmc$	$\rho 4_2/mcm$	$v 4/mmm$
$p4/mmm$	<sup>1</sup> $P4/mmm$	<sup>2</sup> $P4/mcc$	<sup>9</sup> $P4_2/mmc$	<sup>10</sup> $P4_2/mcm$	$p\ v 4/mmm$
$p4/nbm$	<sup>3</sup> $P4/nbm$	<sup>4</sup> $P4/nnc$	<sup>11</sup> $P4_2/nbc$	<sup>12</sup> $P4_2/nmm$	$p\ v 4/nbm$
$p4/mbm$	<sup>5</sup> $P4/mbm$	<sup>6</sup> $P4/mnc$	<sup>13</sup> $P4_2/mbc$	<sup>14</sup> $P4_2/nmm$	$p\ v 4/mbm$
$p4/nmm$	<sup>7</sup> $P4/nmm$	<sup>8</sup> $P4/ncc$	<sup>15</sup> $P4_2/nmc$	<sup>16</sup> $P4_2/ncm$	$p\ v 4/nmm$
$v4/mmm$	$v\ \rho 4/mmm$	$v\ \rho 4/mcc$	$v\ \rho 4_2/mmc$	$v\ \rho 4_2/mcm$	$V 4/mmm$

the last symbol  $vG$  is the symbol of the point-like layer group – it is  $\mathbf{u}^{(\alpha)} \equiv \mathbf{0}$  in both cases.

The space groups on the intersections of rows and columns correspond to systems of non-primitive translations  $\mathbf{u}_G^{(\alpha,\beta)} = \mathbf{u}_G^{(\alpha)} + \mathbf{u}_G^{(\beta)}$ ; the group  $PG$  in the left upper corner of the central table is the symmorphic space group and the group  $VG$  in the right lower corner is the point-like space group – it is  $\mathbf{u}_G^{(\alpha,\beta)} \equiv \mathbf{0}$  in both cases.

Groups in the last column with the lattice  $p\rho$  are the layer-like space groups, whose system of non-primitive translations has trivial components in the direction of the  $c$  axis and components corresponding to the layer group heading the row. The name layer-like space groups is justified by the fact that each  $ab$  plane has the symmetry of this layer group.

Groups in the last row with the lattice  $v\rho$  are the rod-like space groups, whose system of non-primitive translations has trivial components in the direction of the  $ab$  plane and components corresponding to the rod group heading the column. The name rod-like space groups is justified by the fact that each  $c$  line has the symmetry of this rod group. The group  $VG$  in the right lower corner is the point-like space group. This name is justified by the fact that each point  $P$  has the symmetry  $G_p$ .

The tables allow the constructive interpretation in which rod and layer groups combine into space groups as well as the analytical interpretation in which the space groups split into respective rod and layer groups which are the factor groups.

Let us now recall that the choice of the system of non-primitive translations  $\mathbf{u}_G(g) + \varphi(g, \mathbf{s})$  instead of  $\mathbf{u}_G(g)$  corresponds to a group  $\mathcal{G}(\mathbf{s})$ , which is the group  $\mathcal{G}$  shifted in space by  $\mathbf{s}$ . In our choice of systems of non-primitive translations for rod groups, we assume that the line which is left invariant passes through the origin, in the case of layer groups we assume that the plane which is left invariant passes through the origin. This means that chosen systems of non-primitive translations for rod groups do not contain components in  $V(\mathbf{a}, \mathbf{b})$ , for layer groups they do not contain components in  $V(\mathbf{c})$ . Such components may exist but, if they do, they are equivalent to shift functions so that respective rod and layer groups leave invariant lines or planes which do not pass through the origin.

We assume in the proposed system of unified symbols that the systems of non-primitive translations for rod and layer groups are chosen so that they form an additive group; then the systems of non-primitive translations of the space groups form also an additive group – a direct sum of the two groups.

Let  $\mathbf{u}_G^{(\alpha)}(g) \in V(\mathbf{a}, \mathbf{b})$  and  $\mathbf{u}_G^{(\beta)}(g) \in V(\mathbf{c})$  be the systems of non-primitive translations for chosen standards of a layer group  $\mathcal{L}^{(\alpha)}$  and rod group  $\mathcal{R}^{(\beta)}$ , so that the system of non-primitive translations  $\mathbf{u}_G^{(\alpha)}(g) + \mathbf{u}_G^{(\beta)}(g)$  defines the standard space group  $\mathcal{G}^{(\alpha, \beta)}$ . The addition of shift functions  $\varphi(g, \mathbf{s}_1) \in V(\mathbf{a}, \mathbf{b})$ ,  $\varphi(g, \mathbf{s}_2) \in V(\mathbf{c})$  changes the layer group into  $\mathcal{L}^{(\alpha)}(\mathbf{s}_1)$ , the rod group into  $\mathcal{R}^{(\beta)}(\mathbf{s}_2)$  and the space group into  $\mathcal{G}^{(\alpha, \beta)}(\mathbf{s}_1 + \mathbf{s}_2)$ . Hence, in the charts in Tables 9 and 10, an addition of a shift to a rod group leads to an addition of the same shift in all space groups of the column, headed by this rod group. Analogously, an addition of a shift to a layer group leads to an addition of the same shift to all space groups of the row, headed by this layer group.

Last but not least. A long time ago, it was observed by K. Lonsdale and commented on by Cochran (1952) that certain space groups have the same diagrams as certain layer groups. These are the groups with a trivial system of non-primitive translations in the direction of  $V(\mathbf{c})$ , they appear in the first column of the space groups in our charts and their Hermann–Mauguin symbols differ from those of layer groups only by the lattice symbol  $P$  instead of  $p$ . Quite analogously, we can observe diagrams of rod groups in diagrams of certain space groups if we encircle the origin (in some cases they are located at another point; in our interpretation of Hermann–Mauguin symbols they will always be related to the origin). These are the space groups with a trivial system of non-primitive translations in the direction of  $V(\mathbf{a}, \mathbf{b})$ , they appear in the first row of the space groups in our charts and their Hermann–Mauguin symbols differ from those of rod groups only by the lattice symbol  $P$  instead of  $p$ . In a geometrical interpretation, there exists a plane which displays the full layer symmetry in the first case, a line which displays the full rod symmetry in the second case. This is in analogy to symmorphic space groups which display the full point symmetry at a certain

point, usually the origin (in our interpretation it will always be the origin).

We suggested that reducible space groups with decomposable lattices should be classified into layer classes (the rows) and rod classes (the columns) and to say that the space groups of the first column are symmorphic representatives of layer classes, the space groups of the first row are symmorphic representatives of rod classes (Kopský, 1989b, 1993a).

Projections of space groups onto layer and rod groups can also be deduced from the diagrams. If we omit all fractions indicating the height of symmetry elements, replace screw axes perpendicular to the plane of the diagram by ordinary axes, dotted lines by full lines ( $c \rightarrow m$ ) and dash-dotted by dashed lines ( $n \rightarrow a$  or  $b$ ), we obtain the diagram of the corresponding layer group. Analogously, if we move all symmetry elements to the origin leaving their heights, replace the  $2_1$  axes in the plane by ordinary twofold axes, dashed lines by full ones ( $a$  or  $b \rightarrow m$ ), dash-dotted by dotted lines ( $n \rightarrow c$ ) and planes parallel to diagrams by planes, leaving their heights, we obtain the diagram of corresponding rod group.

## 8. Conclusions

There are three new points in the proposed system. (i) To take the location of groups into account in their Hermann–Mauguin symbols. (ii) To correlate Hermann–Mauguin symbols of reducible space groups with those of subperiodic groups. (iii) To extend the standards to groups with semi-continuous and continuous lattices. All three points are justified by applications in theories of material physics. To complete the unified system of Hermann–Mauguin symbols, we have to consider cases of reducible/indecomposable lattices of space (layer) groups where factorization has certain specific features. We shall also extend the system to non-crystallographic and magnetic groups.

## APPENDIX A

Inasmuch as Lemma 1 and the composition law of isometries in the form of Seitz symbols constitute the background of the theory of Euclidean groups, it is appropriate to prove it.

*Proof:* Let  $\alpha : E(n) \rightarrow E(n)$  be an isometry of  $E(n)$  and  $P \in E(n)$  its arbitrary point. Any point  $X \in E(n)$  is expressed as  $X = P + \mathbf{x}$ ,  $\mathbf{x} \in V(n)$ . The isometry  $\alpha$  sends the chosen point  $P$  to  $P' = \alpha P$  and any other point  $X$  to  $X' = \alpha X$ . This point is expressed as  $X' = P' + \mathbf{x}'$  with reference to the point  $P'$ . According to the definition of isometries, the distances  $X - P = |\mathbf{x}|$  and  $X' - P' = |\mathbf{x}'|$  must be equal and hence  $\mathbf{x}' = g\mathbf{x}$ , where  $g \in \mathcal{O}(n)$ . Hence  $X' = \alpha X = P' + g\mathbf{x} = P + (P' - P) + g\mathbf{x}$ . Finally, we obtain

$$\alpha X = P + g\mathbf{x} + \mathbf{t},$$

where  $\mathbf{t} = P' - P$ .

If  $\mathbf{t} = \mathbf{0}$ , operation  $\alpha$  is evidently the rotation of  $E(n)$  about  $P$  which we denote by  $\{g|\mathbf{0}\}_P$ , while  $\mathbf{t} = P' - P$  is a shift of the space  $E(n)$  by  $\mathbf{t}$ . We combine both operations into one in the

Seitz symbol  $\alpha = \{g|\mathbf{t}\}_P$ , so that  $\{g|\mathbf{t}\}_P X = P + g\mathbf{x} + \mathbf{t}$ . Applying successively  $\{g|\mathbf{t}_g\}_P$  and  $\{h|\mathbf{t}_h\}_P$  to an arbitrary point  $X$ , we obtain

$$\{g|\mathbf{t}_g\}_P \{h|\mathbf{t}_h\}_P X = \{g|\mathbf{t}_g\}_P (P + h\mathbf{x} + \mathbf{t}_h) = P + gh\mathbf{x} + g\mathbf{t}_h + \mathbf{t}_g$$

from where the multiplication law of Seitz symbols follows.

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