Unified system of Hermann-Mauguin symbols for groups of material physics

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1. Brief history and current status of symbols

Most of mathematicians who specialize in some branch of group theory would be surprised to hear that groups are of specific importance in physics. Actually, the group theory is connected even 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 special relativity theory, the law of the conservation of energy-momentum tensor also follows from Minkowski's metric of space-time.

Groups are a mathematical tool for consideration of symmetry and its consequences also in material physics. The point groups were originally introduced in connection with classification of the external shape of monocrystals into so-called Hessel-Gadolin classes. Later on, Fedorov and Schoenflies derived independently the 230 types of possible space symmetries of crystals. Neither of these two authors completely succeeded on the first attempt, but 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 has been 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 the first volume of the International Tables for Crystallography under the title Vol. A: Space Group Symmetry. 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 these Tables in 1930, crystallography developed into a specific branch of physical science, the importance of which can be hardly overestimated. Technological applications of crystals belong to pillars of modern civilization, especially in communication technique and it is not an exaggeration if we claim that crystals helped to change this world positively in many aspects. The number of known crystal structures goes today to millions and it is therefore important that there exist generally approved and used standards for their description as given in Vol. A of the International Tables.

Consideration of magnetic properties and of crystals with atoms (or ions) which carry magnetic momentum requires introduction of magnetic point and space groups. The magnetic point groups are sometimes called Heesch groups because they were derived by Heesch already in 1930 as the three-dimensional groups of four dimensional space. In 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 Russian literature. At the moment we can assume that these symbols are generally 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 material physics and even all groups which deserve to be called "crystallographic groups". There exist chemical compounds with symmetries which are not crystallographic and solid state was found to form also so-called quasicrystals whose description requires noncrystallographic groups. Since there is no periodicity, the symmetries of molecules are usually called the point groups. Application of group theory is also not limited by the description of structures. The most powerful use of groups lies in applications of the theory of group representations.

The International Tables for Crystallography were prepared by crystallographers and they 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 which spread over 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 structure is, in a given transition, identical up to orientation and shift in space. Consideration of boundaries constitutes now a subject which is known under the name of Bicrystallography. 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 were historically derived and rederived under different names since the first decades of past century and various symbols were invented for their classification. Eventually there were introduced standards of these groups in a manner analogous to standards of space groups in Vol. E: Subperiodic groups of the International Tables for crystallography. Comparative tables of symbols used throughout the time by various authors, given in this volume, show that there were introduced at least 5 types of symbols for frieze groups, 9 for rod groups and 25 types of symbols for layer groups. Hermann-Mauguin types of symbols for layer groups were introduced and tables analogous to those for the space groups 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, Krause & Grell (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 factor groups of reducible space groups (Kopský, 1986; 1989a,b; 1993a, Fuksa and Kopský, 1993; see also section 5).

Both volumes A and E of the *"International tables for crystallography"* are restricted to the description of only those groups of isometries which are crystallographic and whose translation subgroups are discrete. On the other hand, problems of material physics involve groups with continuous or semicontinuos translation subgroups (lattices in crystallographic terminology) as well as groups of non-crystallographic character. Though ideal crystals have always 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 consideration of *"ferroic"* phase transitions. In this case, it is appropriate to consider the symmetry as a group whose lattice is continuous. In consideration of domain walls or twin boundaries in the same approximation, we need to consider layer groups whose lattice is also continuous. In this connection, it is necessary to amend the usual meaning of terms crystallographic and space groups (see section 3). We shall consider here all cases in which the point and translation subgroups are either discrete, semicontinuous or continuous. The site point groups and point groups will be considered in more detail in the lecture on tensor calculus.

2. Elementary theory of Euclidean groups.

The fact that the Universe in 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 metrics 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 $|\mathbf{x}| = \sqrt{(\mathbf{x}, \mathbf{x})}$. 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 δ_{ij}, known as Kronecker delta, equals 1 just 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 $V(n)$ is expressed as:

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

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 $|\mathbf{x}| = \sqrt{\sum_{i=1}^n x_i^2}$. 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, $Y \in E(n)$ which is written formally as $\mathbf{x} = Y - X$ and the norm of vector $|\mathbf{x}| = \sqrt{\sum_{i=1}^n (y_i - x_i)^2}$ is equal to distances of these pairs of vectors.

A mapping $g : V(n) \longrightarrow V(n)$ of the space $V(n)$ onto itself (a bijection) or on its proper subspace (an injection) is called linear if

$$g(a\mathbf{x} + b\mathbf{y}) = ag\mathbf{x} + bg\mathbf{y}.$$

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} as well is 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 $\mathcal{G}V(n)$, called the general linear group on $V(n)$.

A linear mapping $g : V(n) \longrightarrow V(n)$ 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 $\mathcal{G}V(n)$. 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 again into orthonormal bases because they do not change the scalar products. Linear mappings can be expressed by $n \times n$ matrices according to

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

Thus the choice of a basis $\{\mathbf{e}_i\}_{i=1}^n$ defines an isomorphism of the group $\mathcal{G}V(n)$ 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 $O(n)$ 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 $(x_1, x_2, \ldots, x_n)$ 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 $(P; \{\mathbf{e}_i\}_i^n)$.

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 which 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 symbol of isometries which bear the name of Seitz. Such a symbol, for an isometry which 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:

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

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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

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

where

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

is 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 which operates in a certain manner with reference to point $Q = P + \mathbf{s}$ is expressed by 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 of textbooks on the assumption that the origin is fixed. In our consideration, the distinction of Seitz symbols with reference to different origins is essential.

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

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

From this result we obtain 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 either a point $P + \mathbf{s}_l$, line or plane passing through this point, or the whole space. In the first case, $V_l(g) = V(3)$, the only allowed translation $\mathbf{t}_f = \mathbf{0}$ and the element $\{g|\mathbf{t}\}_P$ 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 also 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 Seitz symbol.

Let us finally comment the choice of subscripts f and l which stand for 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 translation $\{e|\mathbf{t}\}$. 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

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

According to the theory of normal subgroups there exists a homomorphism which maps the group $\mathcal{E}(n)$ onto the factor group $\mathcal{E}(n)/V(n)$ which is the group $\mathcal{O}(n)$. Here $V(n)$ 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). We denote this homomorphism by $\sigma : \mathcal{E}(n) \longrightarrow \mathcal{O}(n)$, so that $\sigma(\{g|\mathbf{t}\}_P) = g$. It is Ker $\sigma(\mathcal{E}(n)) = V(n)$ and Im $\sigma(\mathcal{E}(n)) = \mathcal{O}(n)$.
Remark: An affine transformation of $E(n)$ is, by definition, any transformation which 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 $g \in \mathcal{G}V(n)$.

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:

(i) g are elements of a group $G \subseteq \mathcal{O}(n)$ acting on the vector space $V(n)$ - this is 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 $T_G \trianglelefteq \mathcal{G}$ (the symbol $\trianglelefteq$ 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) $\mathbf{u}_G : g \longrightarrow \mathbf{u}_G(g) \in V(n)/T_G$ is a function from G to the fundamental region $V(n)/T_G$ which satisfies 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:

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

In particular, for the whole 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 nonprimitive translations", the functions $\mathbf{w}_G(g,h)$ as the "factor systems". The systems of nonprimitive translations for the same group with reference to different origins P differ by a shift function $\varphi(g,\mathbf{s})$. Quite generally, any function $\mathbf{u}_G(g) : G \longrightarrow V(n)$, which satisfies 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 $\mathbf{t}(g) : G \longrightarrow T_G$ has it too and defines the same group $\mathcal{G}$. To achieve uniqueness of relationship between groups and systems of nonprimitive translations, we therefore restrict $\mathbf{u}_G(g)$ to the fundamental region $V(n)/T_G$ of T_G.

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.

Systems of nonprimitive translation, factor systems and shift functions appear in two very exacting papers by Ascher & Janner (1965, 1968/69) on space groups in arbitrary dimensions, published years ago, in which the theory of space groups in arbitrary dimensions is treated on the ground of the theory of *"cohomology groups"*. Our approach is a plain version of this theory extended to subperiodic and other Euclidean groups. The author should acknowledge a series of lectures given by recognized Czech specialist on abelian groups, Prof. L. Procházka from Charles University, 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.

The fundamental theorem on arithmetic classes

We shall consider now 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". All groups of the "arithmetic class" will be 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 be then 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, 1993 b). 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 nonprimitive 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. Check that all systems of nonprimitive 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 nonprimitive 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 introduce 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 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 which visualize the group, the parameters of T_G, which are the vectors $(\mathbf{a}, \mathbf{b}, \mathbf{c})$ of crystallographic basis, define the frame in which we draw the diagram. Each system of nonprimitive 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 nonprimitive 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 which fit the frame. Groups with different labels α, β are not necessarily of different space group type.

3. Reducibility and decomposability of Euclidean groups

In most textbook 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 group 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 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 needs 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 combination $a_1\mathbf{x}_1 + a_2\mathbf{x}_2 + \ldots + a_m\mathbf{x}_m$ of any set of its vectors $\mathbf{x}_1$, $\mathbf{x}_2$, $\ldots$, $\mathbf{x}_n$ with coefficients a_i from a number field. The term field means that a 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 the set of these vectors is called the 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 linear combination $n_1\mathbf{x}_1 + n_2\mathbf{x}_2 + \ldots + n_m\mathbf{x}_n$ of any set of its vectors $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n$ 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 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 which do not form a basis though their number equals the rank.

We shall now briefly describe what it means in the 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 even not 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 cubic system. If we consider now 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 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 subspace $V(\mathbf{a}, \mathbf{b})$, $V(\mathbf{c})$, 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 $V(n) = V(k_1) \oplus V(k_2)$. Let further $\sigma_1 : V(n) \longrightarrow V(k_1)$ and $\sigma_2 : V(n) \longrightarrow V(k_2)$ be the projections of the space $V(n)$ onto its G-invariant subspaces $V(k_1)$ 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:

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

where

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

and

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

Vectors $\mathbf{d}_i$, $i = 2, \ldots, p$ here are the centring vectors and $\mathbf{d}_{1i} = \sigma_1 \mathbf{d}_i$, $\mathbf{d}_{2i} = \sigma_1 \mathbf{d}_i$ 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 reductions and decompositions are given in Table 1.1. and Table 1.2., 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 after Table 1.2. Both tables are complemented with symbols for lattices of semicontinuous or continuous character in respective dimensions. Table 1.1. actually applies also to decompositions or reductions of lattices of layer groups.

Table 1.1.

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

Oblique system:			
Any basis vectors **a**, **b**:			
All reductions inclined		T^o_{G1}	T^o_{G2}
p:	$T(\mathbf{a}) \oplus T(\mathbf{b})$	p_a	p_b
Rectangular system:			
All reductions orthogonal		T^o_{G1}	T^o_{G2}
p:	$T(\mathbf{a}) \oplus T(\mathbf{c})$	p_a	p_b
c:	$T(\mathbf{a}) \oplus T(\mathbf{b})[\mathbf{0} \cup (\mathbf{a}+\mathbf{b})/2]$	$\mathsf{p}_{a/2}$	$\mathsf{p}_{b/2}$

List of the meaning of symbols:

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

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. Table 1.1. shows the reduction or decomposition of crystallographic lattices. We consider also lattices which contain continuous components. There are the following types of such lattices in two dimensions:

$\mathsf{p}_a\mathsf{v}_b = T_G(\mathbf{a}) \oplus V_G(\mathbf{b})$, or $\mathsf{v}_a\mathsf{p}_b = V_G(\mathbf{a}) \oplus T_G(\mathbf{b})$, and
$V(\mathbf{a}, \mathbf{b})$.

Lattices $\mathsf{p}_a\mathsf{v}_b$ and $\mathsf{p}_a\mathsf{v}_b$ are invariant only under the action of plane groups of oblique or rectangular system. 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 for lattices of layer groups in which case the invariance refers to three-dimensional point groups.

Table 1.2.

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

Triclinic system:			
Any basis vectors **a**, **b**, **c**			
All reductions inclined		T^o_{G1}	T^o_{G2}
P:	$T(\mathbf{a},\mathbf{b}) \oplus T(\mathbf{c})$	p_{ab}	p_c
Monoclinic system:			
Orthogonal reduction, unique axis **c**:		T^o_{G1}	T^o_{G2}
P:	$T(\mathbf{a},\mathbf{b}) \oplus T(\mathbf{c})$	p_{ab}	p_c
A:	$T(\mathbf{a},\mathbf{b}) \oplus T(\mathbf{c})[\mathbf{0} \cup (\mathbf{b}+\mathbf{c})/2]$	$p_{a,b/2}$	$\mathsf{p}_{c/2}$
B:	$T(\mathbf{a},\mathbf{b}) \oplus T(\mathbf{c})[\mathbf{0} \cup (\mathbf{a}+\mathbf{c})/2]$	$p_{a/2,b}$	$\mathsf{p}_{c/2}$
I:	$T(\mathbf{a},\mathbf{b}) \oplus T(\mathbf{c})[\mathbf{0} \cup (\mathbf{a}+\mathbf{b}+\mathbf{c})/2]$	c_{ab}	$\mathsf{p}_{c/2}$
Inclined reduction, unique axis **a**:		T^o_{G1}	T^o_{G2}
P:	$T(\mathbf{a},\mathbf{b}) \oplus T(\mathbf{c})$	p_{ab}	p_c
C:	$T[(\mathbf{a}+\mathbf{b})/2, (\mathbf{a}-\mathbf{b})/2] \oplus T(\mathbf{c})$	c_{ab}	p_c
B:	$T(\mathbf{a},\mathbf{b}) \oplus T(\mathbf{c})[\mathbf{0} \cup (\mathbf{a}+\mathbf{c})/2]$	$p_{a/2,b}$	$\mathsf{p}_{c/2}$
I:	$T(\mathbf{a},\mathbf{b}) \oplus T(\mathbf{c})[\mathbf{0} \cup (\mathbf{a}+\mathbf{b}+\mathbf{c})/2]$	c_{ab}	$\mathsf{p}_{c/2}$
Inclined reduction, unique axis **b**:		T^o_{G1}	T^o_{G2}
P:	$T(\mathbf{a},\mathbf{b}) \oplus T(\mathbf{c})$	p_{ab}	p
C:	$T[(\mathbf{a}+\mathbf{b})/2, (\mathbf{a}-\mathbf{b})/2] \oplus T(\mathbf{c})$	c_{ab}	p
A:	$T(\mathbf{a},\mathbf{b}) \oplus T(\mathbf{c})[\mathbf{0} \cup (\mathbf{b}+\mathbf{c})/2]$	$p_{a,b/2}$	$\mathsf{p}_{c/2}$
I:	$T(\mathbf{a},\mathbf{b}) \oplus T(\mathbf{c})[\mathbf{0} \cup (\mathbf{a}+\mathbf{b}+\mathbf{c})/2]$	c_{ab}	$\mathsf{p}_{c/2}$
Orthorhombic system:			
All reductions orthogonal:		T^o_{G1}	T^o_{G2}
P:	$T(\mathbf{a},\mathbf{b}) \oplus T(\mathbf{c})$	p_{ab}	p_c
C:	$T[(\mathbf{a}+\mathbf{b})/2, (\mathbf{a}-\mathbf{b})/2] \cup T(\mathbf{c})$	c_{ab}	p_c
B:	$T(\mathbf{a},\mathbf{b}) \oplus T(\mathbf{c})[\mathbf{0} \cup (\mathbf{a}+\mathbf{c})/2]$	$p_{a/2,B}$	$\mathsf{p}_{c/2}$
A:	$T(\mathbf{a},\mathbf{b}) \oplus T(\mathbf{c})[\mathbf{0} \cup (\mathbf{b}+\mathbf{c})/2]$	$p_{a,b/2}$	$\mathsf{p}_{c/2}$
F:	$T[(\mathbf{a}+\mathbf{b})/2, (\mathbf{a}-\mathbf{b})/2] \oplus T(\mathbf{c})[\mathbf{0} \cup (\mathbf{a}+\mathbf{c})/2]$	$p_{a/2,b/2}$	$\mathsf{p}_{c/2}$
I:	$T(\mathbf{a},\mathbf{b}) \oplus T(\mathbf{c})[\mathbf{0} \cup (\mathbf{a}+\mathbf{b}+\mathbf{c})/2]$	c_{ab}	$\mathsf{p}_{c/2}$

Table 1.2 (continued)

Tetragonal system:			
All reductions orthogonal:		T^o_{G1}	T^o_{G2}
P:	$T(\mathbf{a},\mathbf{b}) \cup T(\mathbf{c})$	p_{ab}	p_c
I:	$T(\mathbf{a},\mathbf{b}) \oplus T(\mathbf{c})[\mathbf{0} \cup (\mathbf{a}+\mathbf{b}+\mathbf{c})/2]$	$\widehat{p}_{ab}$	$\mathsf{p}_{c/2}$
Hexagonal family:			
All reductions orthogonal:			
Single Z-decomposition (P) only in hexagonal system			
Either Z-decomposition (P) or Z-reduction (R) in trigonal system.			
		T^o_{G1}	T^o_{G2}
P:	$T(\mathbf{a},\mathbf{b}) \oplus T(\mathbf{c})$	p_{ab}	p_c
R_1 (inverse setting):	$T(\mathbf{a},\mathbf{b}) \oplus T(\mathbf{c})[\mathbf{0} \cup (2\mathbf{a}+\mathbf{b}+\mathbf{c})/3 \cup (\mathbf{a}+2\mathbf{b}+2\mathbf{c})/3]$	$\widehat{p}_{1/3}$	$\mathsf{p}_{c/3}$
R_2 (reverse setting):	$T(\mathbf{a},\mathbf{b}) \oplus T(\mathbf{c})[\mathbf{0} \cup (\mathbf{a}+2\mathbf{b}+\mathbf{c})/3 \cup (2\mathbf{a}+\mathbf{b}+2\mathbf{c})/3]$	$\widehat{p}_{1/3}$	$\mathsf{p}_{c/3}$

List of the meaning 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 orthorhombic system
$\widehat{p}_{ab} = T(\mathbf{a}) \oplus T((\mathbf{a}+\mathbf{b})/2] = T[(\mathbf{a}+\mathbf{b})/2,(\mathbf{a}-\mathbf{b})/2]$, in tetragonal system
$\widehat{p}_{1/3} = T[(2\mathbf{a}+\mathbf{b})/3,(\mathbf{a}+2\mathbf{b})/3]$,
$\mathsf{p}_c = T(\mathbf{c})$, $\mathsf{p}_{c/2} = T(\mathbf{c}/2)$, $\mathsf{p}_{c/3} = T(\mathbf{c}/3)$.

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 which decompose under the action of certain point groups. We denote them as follows:

$p_{ab}\mathsf{v}_c = T_G(\mathbf{a},\mathbf{b})) \oplus V_G(\mathbf{c})$, or $v_{ab}\mathsf{p}_c = V_G(\mathbf{a},\mathbf{b}) \oplus T_G(\mathbf{c})$, 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 $D_{\infty,z} = \infty_z/m_z mm$.

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.

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 $V_d(k_d) =< T_d >_R$ is the linear envelope of the discrete part and $V_l(d)$ is the complement to the linear envelope $< T_G >_R$, called here the "space of missing translations". In general, we do not require that this complement be orthogonal to $< T_G >_R$ 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 $k_d > 0$, $k_c = 0$.

Up to three dimensional lattices we then have the following lattice types:

$n - d = k_t = 1$ $\quad\mathsf{p}$ discrete, v continuous

$n - d = k_t = 2$ $\quad p$, c discrete, v continuous, pv semicontinuous

$n - d = k_t = 3$ $\quad P$, I, F, $A \approx B \approx C$, R discrete Bravais lattices, V continuous, $p\mathsf{v}$, $c\mathsf{v}$, $\mathsf{p}v$ semicontinuous.

The letters v, v, and V have the meaning of vector spaces of dimensions one, two, and three. We anticipate the use of script lower case fonts instead of sans serif fonts p and v for the discrete and continuous one-dimensional lattice. 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 v.
Point-like plane and layer groups for groups with the lattice v.
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 pv.
Layer-like space groups for groups with lattices $p\mathsf{v}$ or $c\mathsf{v}$.
Rod-like space groups for groups with the lattice $\mathsf{p}v$.

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 p of the lattice has the symmetry of the same rod group.

4. Amendments of classical terminology

Space, subperiodic and site-point groups

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

$\boxed{\text{The 1st amendment of standard terminology}}$

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 $V_t(k_t)$; the number $d = n - k_t$ 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".
$d = 1$, $k_t = 1$ "frieze groups".

Dimension 3: $n = 3$, $d = 0$ "space groups".
$d = 1$, $k_t = 2$ "layer groups".
$d = 2$, $k_t = 1$ "rod groups".

Dimension 4: $n = 4$, $d = 1$, $k_t = 3$ "magnetic space groups (Shubnikov groups)".
$d = 2$, $k_t = 2$ "magnetic layer groups".
$d = 3$, $k_t = 1$ "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 nontraditional meaning is already in use for so-called *"quasicrystallographic space groups"* and it is an adequate and natural terminology (Rokhsar et al, 1988).

$\boxed{\text{The 2nd amendment of standard terminology:}}$

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: A 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 in standard terminology: *Example:* The point-like space group $Vm\overline{3}m$ is the symmetry of a crystal of the point symmetry $m\overline{3}m$ 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*. Sec. 15 of Vol. A by Koch & Fischer; since 2nd edition, 1987; see also more detailed consideration of translation normalizer by Kopský, 1993b).

5. Factorization of reducible 3d 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 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. Quite general situation is considered by Kopský (1986), reducibility of 3d space groups by Kopský (1988b, 1989a,b, 1993a), Fuksa and Kopský (1993). Detailed theory is based on application of the concept of subdirect products for reducible point groups) and of subdirect sums for translation subgroups (see Kopský, 1993a). 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 analyze the case of reducible 3d space groups. In an analytic approach we show that reducibility implies the existence of a layer and rod group as factor groups of the space group. In constructive approach we show, how a reducible space group can be assigned to a pair of layer and rod group 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 nonprimitive 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 $\mathcal{R}$:

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

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:

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

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 group 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 $(G, T(\mathbf{c}))$:

$$\mathcal{L}^{(\alpha)}(\mu) = \{G, T(\mathbf{a}, \mathbf{b}), P, \mathbf{u}_{G1}^{(\alpha)}(g) + \varphi(g, \mu)\}, \quad \mathcal{R}^{(\beta)}(\nu) = \{G, T(\mathbf{c}), P, \mathbf{u}_{G2}^{(\beta)}(g) + \varphi(g, \nu)\}$$

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

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

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:

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

which corresponds to:

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

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 2: 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 nonprimitive translations which is trivial.

There are three ways to illustrate the relationship between reducible space groups and respective layer and rod groups:
(i) by tables of systems of nonprimitive translations; two examples are given in Table 3.
(ii) by tables of Hermann-Mauguin symbols; here we can observe either how 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.
(iii) by comparison of group diagrams.

The next Table 2. gives a chart of groups of reducible geometric class including groups with semicontinuous and continuous lattices.

Table 2. Reducibility tables for 3d space groups

Primitive type and decomposable cases:

Geometric class	**rod** groups with *discrete* lattice p_c	**rod** group with *continuous* lattice v_c
layer groups with *discrete primitive* lattice p_{ab}	reducible **space** groups with *primitive* lattice P	**layerlike space** groups with *semicontinuos* lattice $p_{ab}\mathsf{v}_c$
layer groups with *discrete centred* lattice c_{ab}	reducible **space** groups with *base centred* lattice in C setting C	**layerlike** space groups with *semicontinuos* lattice $c_{ab}\mathsf{v}_c$
layer group with *continuous* lattice v_{ab}	**rodlike space** groups with *semicontinuous* lattice $v_{ab}\mathsf{p}_c$	**pointlike space** group with *continuous* lattice V

Centred type - reducible/indecomposable cases:

Geometric class	**rod** groups: homomorphic projection of centred space group by σ_{ab}
layer groups: homomorphic projection of centred space group by σ_c	reducible **space** groups with *centred* lattice: setting A, B of a *base centred* type or one of the F, I types; several groups may lie on the intersection of a row and of a column

$$\sigma_c(A) = p_{a,b/2},\ \sigma_c(B) = p_{a/2,b},\ \sigma_c(F) = p_{a/2,b/2},\ \sigma_c(I) = \widehat{p}_{a,b} \ \text{ or } \ c_{ab}$$
$$\sigma_{ab}(A) = \sigma_{ab}(B) = \sigma_{ab}(F) = \sigma_{ab}(I) = \mathsf{p}_{c/2}$$

Alternative symbols, if any.

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Table 3. Systems of nonprimitive translations

Geometric class $C_{4h} - 4/m$:

Arithmetic classes:	$4/m\mathsf{p}$	$4/mp$	$4/mP$
Cohomology groups:	$C_2 = C(\alpha_2)$;	$C_2 = C(\alpha_1)$;	$C_2^2 = C(\alpha_1, \alpha_2)$.

Cohomology element	Arithmetic class	Group type	4_z	2_z	4_z^{-1}	i	$\overline{4}_z$	m_z	$\overline{4}_z^{-1}$	Correlation with space groups according to IT 1983/87	**Origin choice:** 1	2
ε_2	$4/m\mathsf{p}$	$\mathsf{p}4/m$	$\mathbf{0}$	$\mathbf{0}$	$\mathbf{0}$	$\mathbf{0}$	$\mathbf{0}$	$\mathbf{0}$	$\mathbf{0}$			
α_2	**rod**	$\mathsf{p}4_2/m$	$\mathbf{c}/2$	$\mathbf{0}$	$\mathbf{c}/2$	$\mathbf{0}$	$\mathbf{c}/2$	$\mathbf{0}$	$\mathbf{c}/2$			
ε_1	$4/mp$	$p4/m$	$\mathbf{0}$	$\mathbf{0}$	$\mathbf{0}$	$\mathbf{0}$	$\mathbf{0}$	$\mathbf{0}$	$\mathbf{0}$			
α_1	**layer**	$p4/n$	$\mathbf{0}$	$\mathbf{0}$	$\mathbf{0}$	$(\mathbf{a}+\mathbf{b})/2$	$(\mathbf{a}+\mathbf{b})/2$	$(\mathbf{a}+\mathbf{b})/2$	$(\mathbf{a}+\mathbf{b})/2$			
ε_1		$P4/m$	$\mathbf{0}$	$\mathbf{0}$	$\mathbf{0}$	$\mathbf{0}$	$\mathbf{0}$	$\mathbf{0}$	$\mathbf{0}$	C_{4h}^1	$\mathbf{0}$	-
α_2	$4/mP$	$P4_2/m$	$\mathbf{c}/2$	$\mathbf{0}$	$\mathbf{c}/2$	$\mathbf{0}$	$\mathbf{c}/2$	$\mathbf{0}$	$\mathbf{c}/2$	C_{4h}^2	$\mathbf{0}$	-
α_1	**space**	$P4/n$	$\mathbf{0}$	$\mathbf{0}$	$\mathbf{0}$	$(\mathbf{a}+\mathbf{b})/2$	$(\mathbf{a}+\mathbf{b})/2$	$(\mathbf{a}+\mathbf{b})/2$	$(\mathbf{a}+\mathbf{b})/2$	C_{4h}^3	$\mathbf{a}/2$	$(\mathbf{a}+\mathbf{b})/4$
$\alpha_1\alpha_2$		$P4_2/n$	$\mathbf{c}/2$	$\mathbf{0}$	$\mathbf{c}/2$	$(\mathbf{a}+\mathbf{b})/2$	$(\mathbf{a}+\mathbf{b}+\mathbf{c})/2$	$(\mathbf{a}+\mathbf{b})/2$	$(\mathbf{a}+\mathbf{b}+\mathbf{c})/2$	C_{4h}^4	$\mathbf{a}/2+\mathbf{c}/4$	$(\mathbf{a}+3\mathbf{b})/4$

In this and in the following table we can observe how systems of nonprimitive translations for layer and rod groups combine by addition into systems of nonprimitive translations of reducible space groups with decomposable lattices. The systems of nonprimitive translations are chosen here in such a manner that they constitute an additive group. The last columns correlate this choice with the choice of diagrams in Vol. A. As we can see, especially in the table for geometric class $C_{4v} - 4_z m_x m_{xy}$, the choice of diagrams in Vol. A is not compatible with the requirement that the systems of nonprimitive translation constitute a group. The rules for cases of reducible/indecomposable lattices (centred cases) are slightly more complicated.

Apart from groups listed in these tables there exist groups of the same geometric classes with continuous and semicontinuous lattices. It is not necessary to provide systems of nonprimitive translations for these groups because these systems can be chosen as trivial for the continuous part of the lattice. Thus the systems of nonprimitive translations for point-like rod groups $\mathsf{v}_c G$, point-like layer groups $v_{ab}G$ and point like space groups VG are trivial, while the systems of nonprimitive translations for rod-like space groups $v_{ab}\mathsf{p}_c G$ and layer-like space groups $p_{ab}\mathsf{v}_c G$ are the same as for respective rod groups $\mathsf{p}_c G$ and layer groups $v_{ab}G$.

Geometric class $C_{4v} - 4mm$:

Arithmetic classes: $4mm\mathsf{p}$ $4mmp$ $4mmP$
Cohomology groups: $C_2^2 = C(\alpha_2, \beta_2)$; $C_2 = C(\alpha_1)$; $C_2^3 = C(\alpha_1, \alpha_2, \beta_2)$

Cohomology element	Arithmetic class	Group type	4_z	2_z	4_z^{-1}	m_x	m_{xy}	m_y	$m_{x\overline{y}}$	Correlation with space groups according to IT 1983/87	One origin choice:
ε_2		$\mathsf{p}4mm$	$\mathbf{0}$	$\mathbf{0}$		$\mathbf{0}$	$\mathbf{0}$	$\mathbf{0}$	$\mathbf{0}$		
α_2	$4mm\mathsf{p}$	$\mathsf{p}4_2cm$	$\mathbf{c}/2$	$\mathbf{0}$	$\mathbf{c}/2$	$\mathbf{c}/2$	$\mathbf{0}$	$\mathbf{c}/2$	$\mathbf{0}$		
β_2	**rod**	$\mathsf{p}4_2mc$	$\mathbf{c}/2$	$\mathbf{0}$	$\mathbf{c}/2$	$\mathbf{0}$	$\mathbf{c}/2$	$\mathbf{0}$	$\mathbf{c}/2$		
$\alpha_2\beta_2$		$\mathsf{p}4cc$	$\mathbf{0}$	$\mathbf{0}$	$\mathbf{0}$	$\mathbf{c}/2$	$\mathbf{c}/2$	$\mathbf{c}/2$	$\mathbf{c}/2$		
ε_1	$4mmp$	$p4mm$	$\mathbf{0}$	$\mathbf{0}$	$\mathbf{0}$	$\mathbf{0}$	$\mathbf{0}$	$\mathbf{0}$	$\mathbf{0}$		
α_1	**layer**	$p4bm$	$\mathbf{0}$	$\mathbf{0}$	$\mathbf{0}$	$(\mathbf{a}+\mathbf{b})/2$	$(\mathbf{a}+\mathbf{b})/2$	$(\mathbf{a}+\mathbf{b})/2$	$(\mathbf{a}+\mathbf{b})/2$		
ε		$P4mm$	$\mathbf{0}$	$\mathbf{0}$	$\mathbf{0}$	$\mathbf{0}$	$\mathbf{0}$	$\mathbf{0}$	$\mathbf{0}$	C_{4v}^1	$\mathbf{0}$
α_1		$P4bm$	$\mathbf{0}$	$\mathbf{0}$	$\mathbf{0}$	$(\mathbf{a}+\mathbf{b})/2$	$(\mathbf{a}+\mathbf{b})/2$	$(\mathbf{a}+\mathbf{b})/2$	$(\mathbf{a}+\mathbf{b})/2$	C_{4v}^2	$\mathbf{0}$
α_2		$P4_2cm$	$\mathbf{c}/2$	$\mathbf{0}$	$\mathbf{c}/2$	$\mathbf{c}/2$	$\mathbf{0}$	$\mathbf{c}/2$	$\mathbf{0}$	C_{4v}^3	$\mathbf{0}$
$\alpha_1\alpha_2$	$4mmP$	$P4_2nm$	$\mathbf{c}/2$	$\mathbf{0}$	$\mathbf{c}/2$	$(\mathbf{a}+\mathbf{b}+\mathbf{c})/2$	$(\mathbf{a}+\mathbf{b})/2$	$(\mathbf{a}+\mathbf{b}+\mathbf{c})/2$	$(\mathbf{a}+\mathbf{b})/2$	C_{4v}^4	$\mathbf{a}/2$
$\alpha_2\beta_2$	**space**	$P4cc$	$\mathbf{0}$	$\mathbf{0}$	$\mathbf{0}$	$\mathbf{c}/2$	$\mathbf{c}/2$	$\mathbf{c}/2$	$\mathbf{c}/2$	C_{4v}^5	$\mathbf{0}$
$\alpha_1\alpha_2\beta_2$		$P4nc$	$\mathbf{0}$	$\mathbf{0}$	$\mathbf{0}$	$(\mathbf{a}+\mathbf{b}+\mathbf{c})/2$	$(\mathbf{a}+\mathbf{b}+\mathbf{c})/2$	$(\mathbf{a}+\mathbf{b}+\mathbf{c})/2$	$(\mathbf{a}+\mathbf{b}+\mathbf{c})/2$	C_{4v}^6	$\mathbf{0}$
β_2		$P4_2mc$	$\mathbf{c}/2$	$\mathbf{0}$	$\mathbf{c}/2$	$\mathbf{0}$	$\mathbf{c}/2$	$\mathbf{0}$	$\mathbf{c}/2$	C_{4v}^7	$\mathbf{0}$
$\alpha_1\beta_2$		$P4_2bc$	$\mathbf{c}/2$	$\mathbf{0}$	$\mathbf{c}/2$	$(\mathbf{a}+\mathbf{b})/2$	$(\mathbf{a}+\mathbf{b}+\mathbf{c})/2$	$(\mathbf{a}+\mathbf{b})/2$	$(\mathbf{a}+\mathbf{b}+\mathbf{c})/2$	C_{4v}^8	$\mathbf{0}$

The following set of tables illustrates the principle of the unification of Hermann-Mauguin symbols for groups of the tetragonal geometric classes $G = 422$, $4mm$, $\overline{4}2m$, and $4/mmm$, based on the Schreier law and theorem 2. We consider only the arithmetic classes GP of space groups, where the primitive lattices P decompose into a direct sum $T(\mathbf{a},\mathbf{b},\mathbf{c}) = P = p \oplus \mathsf{p} = T(\mathbf{a},\mathbf{b}) \oplus T(\mathbf{c})$. These classes are specified in the heading and in the left upper corner of each table.

Table 4. Correlation of Hermann-Mauguin symbols for reducible space groups with those of layer and rod groups:

Arithmetic class $422P$

$422P$	$\mathsf{p}422$	$\mathsf{p}4_122$	$\mathsf{p}4_222$	$\mathsf{p}4_322$	$\mathsf{v}422$
$p422$	$^{1}P422$	$^{3}P4_122$	$^{5}P4_222$	$^{7}P4_322$	$p\mathsf{v}422$
$p42_12$	$^{2}P42_12$	$^{4}P4_12_12$	$^{6}P4_22_12$	$^{8}P4_32_12$	$p\mathsf{v}42_12$
$v422$	$v\mathsf{p}422$	$v\mathsf{p}4_122$	$v\mathsf{p}4_222$	$v\mathsf{p}4_322$	$V422$

Arithmetic class $4mmP$

$4mmP$	$\mathsf{p}4mm$	$\mathsf{p}4_2cm$	$\mathsf{p}4cc$	$\mathsf{p}4_2mc$	$\mathsf{v}4mm$
$p4mm$	$^{1}P4mm$	$^{3}P4_2cm$	$^{5}P4cc$	$^{7}P4_2mc$	$p\mathsf{v}4mm$
$p4bm$	$^{2}P4bm$	$^{4}P4_2nm$	$^{6}P4nc$	$^{8}P4_2bc$	$p\mathsf{v}4bm$
$v4mm$	$v\mathsf{p}4mm$	$v\mathsf{p}4_2cm$	$v\mathsf{p}4cc$	$v\mathsf{p}4_2mc$	$V4mm$

Arithmetic class $\overline{4}2mP$

$\overline{4}2mP$	$\mathsf{p}\overline{4}2m$	$\mathsf{p}\overline{4}2c$	$\mathsf{v}\overline{4}2m$
$p\overline{4}2m$	$^{1}P\overline{4}2m$	$^{2}P\overline{4}2c$	$p\mathsf{v}\overline{4}2m$
$p\overline{4}2_1m$	$^{3}P\overline{4}2_1m$	$^{4}P\overline{4}2_1c$	$p\mathsf{v}\overline{4}2_1m$
$v\overline{4}2m$	$v\mathsf{p}\overline{4}2m$	$v\mathsf{p}\overline{4}2c$	$V\overline{4}2m$

Arithmetic class $\overline{4}m2P$

$\overline{4}m2P$	$\mathsf{p}\overline{4}m2$	$\mathsf{p}\overline{4}c2$	$\mathsf{v}\overline{4}m2$
$p\overline{4}m2$	$^{5}P\overline{4}m2$	$^{6}P\overline{4}c2$	$p\mathsf{v}\overline{4}m2$
$p\overline{4}b2$	$^{7}P\overline{4}b2$	$^{8}P\overline{4}n2$	$p\mathsf{v}\overline{4}b2$
$v\overline{4}m2$	$v\mathsf{p}\overline{4}m2$	$v\mathsf{p}\overline{4}c2$	$V\overline{4}m2$

Arithmetic class $4/mmmP$

$4/mmmP$	$\mathsf{p}4/mmm$	$\mathsf{p}4/mcc$	$\mathsf{p}4_2/mmc$	$\mathsf{p}4_2/mcm$	$\mathsf{v}4/mmm$
$p4/mmm$	$^{1}P4/mmm$	$^{2}P4/mcc$	$^{9}P4_2/mmc$	$^{10}P4_2/mcm$	$p\mathsf{v}4/mmm$
$p4/nbm$	$^{3}P4/nbm$	$^{4}P4/nnc$	$^{11}P4_2/nbc$	$^{12}P4_2/nnm$	$p\mathsf{v}4/nbm$
$p4/mbm$	$^{5}P4/mbm$	$^{6}P4/mnc$	$^{13}P4_2/mbc$	$^{14}P4_2/mnm$	$p\mathsf{v}4/mbm$
$p4/nmm$	$^{7}P4/nmm$	$^{8}P4/ncc$	$^{15}P4_2/nmc$	$^{16}P4_2/ncm$	$p\mathsf{v}4/nmm$
$v4/mmm$	$v\mathsf{p}4/mmm$	$v\mathsf{p}4/mcc$	$v\mathsf{p}4_2/mmc$	$v\mathsf{p}4_2/mcm$	$V4/mmm$

The Hermann-Mauguin symbols of the space groups are arranged in the central part of each table. The superscripts are the numerical labels of the respective Schönflies symbols. The first row contains symbols of rod groups of the arithmetic class $G\mathsf{p}$ which correspond to systems of nonprimitive translations $\mathbf{u}^{(\beta)}$; the first symbol $\mathsf{p}G$ is the symbol of the symmorphic rod group, the last symbol $\mathsf{v}G$ 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 nonprimitive translations $\mathbf{u}^{(\alpha)}$; the first symbol pG is the symbol of the symmorphic layer group, 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 nonprimitive 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 $p\mathsf{v}$ are the layer-like space groups, whose system of nonprimitive translations has trivial components in the direction of 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 $v\mathsf{p}$ are the rod-like space groups, whose system of nonprimitive translations has trivial components in the direction of 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.

Notice the manner in which the Hermann-Mauguin symbols of rod and layer groups combine into the Hermann-Mauguin symbols of the space groups (construction approach) or, vice versa, the manner in which the symbol of a space group splits into a pair of symbols of the rod and layer group (analytic approach).

Thus the main axis 4 cannot be screw axis in a layer group but there are ordinary 4-axis and screw axes 4_1, 4_2, 4_3 in rod groups which combine with 4-axis into axes 4, 4_1, 4_2, 4_2 in space groups.

On the other hand, auxiliary axes 2 cannot be screw axes in a rod group and they combine with 2 or 2_1 axis in a rod group into 2 or 2_1-axis in space groups.

The plane, perpendicular to c-axis can be either m or n in a layer group and only m in a rod group, so that they combine into m or n in space groups.

The two auxiliary planes can be either m or b (equivalent to a in tetragonal groups) in layer groups and either m or c in rod groups. According to rules of Hermann-Mauguin symbols they combine into $m \approx (m, m)$, $b \approx (b, m)$ $c \approx (m, c)$, $n \approx (b, c)$ in space groups. In orthorhombic system, the a and b-axes are not equivalent, so that there appear symbols a, b, n in symbols of layer groups while only m and c appear in symbols of rod groups. We have therefore also combinations $a \approx (a, m)$, $b \approx (b, m)$ and $n \approx (a, c) \approx (b, c)$.

Let us now recall, that the choice of the system of nonprimitive 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 nonprimitive 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 nonprimitive 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 nonprimitive translations for rod and layer groups are chosen so that they form an additive group; then the systems of nonprimitive 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 nonprimitive translations for chosen standards of a layer group $\mathcal{L}^{(\alpha)}$ and rod group $\mathcal{R}^{(\beta)}$, so that the system of nonprimitive translations $\mathbf{u}_G^{(\alpha)}(g) + \mathbf{u}_G^{(\beta)}(g)^{(\beta)}$ defines the standard space group $\mathcal{G}^{(\alpha,\beta)}$. The addition of shift functions $\varphi(g, \mathbf{s}_1) \in V(\mathbf{a}, \mathbf{b})$, $\varphi(g, \mathbf{s}_2) \in V(\mathbf{c})$ change 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 tables of Table 4, an addition of a shift to a rod function 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.

This leads to a clash between standard diagrams of rod and layer groups in Vol. E and standards of space groups in Vol. A of the International Tables. Worse than that, it is impossible to choose standards of rod and layer groups to avoid these clashes. This is the consequence of the fact that we understand Hermann-Mauguin symbols as symbols of quite specific groups, including their location. In fact, we propose to use Hermann-Mauguin symbol $\mathcal{G}(\mathbf{s})$ for a group which differs from the group with Hermann-Mauguin symbol $\mathcal{G}$ and consider certain groups $\mathcal{G}$ whose diagrams are not always those from Vol. A, as standards for meaning of the symbols.

Last but not least. A long time ago, it has been observed by K. Lonsdale and commented by Cochran, that certain space groups have the same diagrams as certain layer groups. These are the groups with trivial system of nonprimitive translations in the direction of $V(\mathbf{c})$. Quite analogously, we can observe diagrams of certain rod groups in diagrams of certain space groups. These are the groups with trivial system of nonprimitive translations in the direction of $V(\mathbf{a}, \mathbf{b})$. 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 an analogy to symmorphic space groups which display the full point symmetry at a certain point, usually the origin.

Conclusion: The new point in our system is that we take the location of groups into account. This problem is in particular important in the Scanning Tables of Vol. E, from the viewpoint of a physicist in all problems when we have to consider domain walls or twin boundaries for which the scanning tables are designed. The location problem needs a slightly more detailed analysis with introduction of a few new concepts.

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GI $\star$ KoBo-1 (*Group Informatics.* Kopský, V. & Boček, P., release 1.)
CD ROM Supplement to Vol. D. For Windows 95.

Exercises:

Exercise 1: Find symbols of space groups of arithmetic classes $mm2P$ and $mm2C$ and fill them in the table!

Geometric class C_{2v}:

Orientation $mm2$

Arithmetic classes $mm2P$ and $mm2C$

Decomposition

$mm2$P	$mc2_1$ $cm2_1$ $cc2$	$mm2$
$pma2$ $pbm2$ $pba2$		
$mm2C$		
$cmm2$		
$vmm2$		

Exercise 3: Consider the diagram of the space group $T_h^6 - Pa\overline{3}$. If you rotate this diagram by 90 degrees, you obtain another diagram of this group. There exists no shift which will move this diagram to coincide with the original. Explain the meaning of this sad fact!

Exercise 4: Consider the diagrams of the group $D_{4h}^{15} - P4_2/nmc$ for the two origin choices in Vol. A. How shall we describe these two groups in our system?

Exercise 5: The group D_{2h}^8 is visualized in Vol. A by six different settings to which there correspond abbreviated Hermann-Mauguin symbols $Pcca$, $Pccb$, $Pbab$, $Pbaa$, $Pcaa$ and $Pbca$. Give two possible interpretations of these symbols:

(i) an interpretation in which the symbols mean the same group,

(ii) an interpretation in which the symbols mean different groups with reference to crystallographic basis $(\mathbf{a}, \mathbf{b}, \mathbf{c})$.

Exercise 6: Show that the shift function satisfies Frobenius congruences!

Exercise 7: Show that the trivial system of nonprimitive translations $\mathbf{u}_G(g) \equiv \mathbf{0}$ or $\varphi(g, \mathbf{s})$ corresponds to a symmorphic group!

Exercise 2: Fill the gaps in the decomposition table for arithmetic classes $mmmP$ and $mmmC$!

Geometric class $D_{2h} - mmm$:

Arithmetic classes $mmmP$ and $mmmC$

Decomposition

$mmmP$		mcm			
	$^{1}Pmmm$	$^{5}Pmcm$	$^{5}Pcmm$	$^{3}Pccm$	
$pmmn$			$^{16}Pcmn$	$^{10}Pccn$	
$pbam$	$^{9}Pbam$	$^{16}Pbnm$	$^{16}Pnam$	$^{12}Pnnm$	
$pban$	$^{4}Pban$		$^{6}Pnan$	$^{2}Pnnn$	
	$^{5}Pmma$	$^{11}Pmca$		$^{8}Pcca$	$p\ \ mma$
	$^{5}Pmmb$		$^{11}Pcmb$	$^{8}Pccb$	$p\ \ mmb$
	$^{5}Pmam$	$^{13}Pmnm$	$^{11}Pcam$	$^{7}Pcnm$	$p\ \ mam$
	$^{5}Pbmm$		$^{13}Pnmm$	$^{7}Pncm$	$p\ \ bmm$
pmaa	$^{3}Pmaa$	$^{7}Pmna$		$^{4}Pcna$	
$pbmb$	$^{3}Pbmb$	$^{8}Pbcb$	$^{7}Pnmb$		
$pmab$	$^{11}Pmab$		$^{15}Pcab$	$^{14}Pcnb$	
$pbma$	$^{11}Pbma$	$^{15}Pbca$		$^{14}Pnca$	
		$^{12}Pmnn$	$^{14}Pcan$	$^{6}Pcnn$	man
	$^{7}Pbmn$	$^{14}Pbcn$		$^{6}Pncn$	$p\ \ bmn$
	$^{8}Pbaa$		$^{10}Pnaa$	$^{6}Pnna$	$p\ \ baa$
	$^{8}Pbab$	$^{10}Pbnb$	$^{14}Pnab$	$^{6}Pnnb$	p$vbab$
$mmmC$					
	$^{19}Cmmm$	$^{17}Cmcm$	$^{17}Ccmm$	$^{20}Cccm$	$c\ \ mmm$
$cmma$	$^{21}Cmma$		$^{18}Ccma$	$^{22}Ccca$	
	$^{21}Cmmb$	$^{18}Cmcb$		$^{22}Cccb$	$c\ \ mmb$
$vmmm$			$v\ \ cmm$	$v\ \ ccm$	

Solutions:

Exercise 1:

Geometric class C_{2v}:

Orientation $mm2$

Arithmetic classes $mm2P$ and $mm2C$

Decomposition

$mm2$P	p$mm2$	p$mc2_1$	p$cm2_1$	p$cc2$	v$mm2$
$pmm2$	${}^1Pmm2$	${}^2Pmc2_1$	${}^2Pcm2_1$	${}^3Pcc2$	pv$mm2$
$pma2$	${}^4Pma2$	${}^7Pmn2_1$	${}^5Pca2_1$	${}^6Pcn2$	pv$ma2$
$pbm2$	${}^4Pbm2$	${}^5Pbc2_1$	${}^7Pnm2_1$	${}^6Pnc2$	pv$bm2$
$pba2$	${}^8Pba2$	${}^9Pbn2_1$	${}^9Pna2_1$	${}^{10}Pnn2$	pv$ba2$
$mm2C$					
$cmm2$	${}^{11}Cmm2$	${}^{12}Cmc2_1$	${}^{12}Ccm2_1$	${}^{13}Ccc2$	cv$mm2$
$vmm2$	vp$mm2$	vp$mc2_1$	vp$cm2_1$	vp$cc2$	$Vmm2$

Exercise 3: The following table of systems of nonprimitive translations illustrates the solution.

$e,\ i$	$2_x,\ m_x$	$2_y,\ m_y$	$2_z,\ m_z$		
$\mathbf{0}$	$\mathbf{0}$	$\mathbf{0}$	$\mathbf{0}$	$D_{2h}^1 - Pmmm$	$T_h^1 - Pm\overline{3}$
$\mathbf{0}$	$(\mathbf{a}+\mathbf{b})/2$	$(\mathbf{b}+\mathbf{c})/2$	$(\mathbf{a}+\mathbf{c})/2$	$D_{2h}^{15} - Pbca$	$T_h^6 - Pa\overline{3}$
$\mathbf{0}$	$(\mathbf{a}+\mathbf{c})/2$	$(\mathbf{a}+\mathbf{b})/2$	$(\mathbf{b}+\mathbf{c})/2$	$D_{2h}^{15} - Pcab$	$T_h^6 - Pb\overline{3}$
$\mathbf{0}$	$(\mathbf{b}+\mathbf{c})/2$	$(\mathbf{a}+\mathbf{c})/2$	$(\mathbf{a}+\mathbf{b})/2$	$D_{2h}^2 - Pnnn$	$T_h^2 - Pn\overline{3}$

The table contains for simplicity only nonprimitive translations for the subgroup mmm of the point group $m\overline{3}$. Corresponding orthorhombic subgroups of cubic groups of arithmetic class $m\overline{3}P$ are given in the last but one column, the groups of this class in the last column. The group $Pb\overline{3}$ is just another setting (in crystallographic language) of the group $Pa\overline{3}$. Without this group, the table of systems of nonprimitive translations will not be complete. Both orthorhombic and cubic groups in the last row correspond to origin choice 2.

Exercise 2:

Geometric class $D_{2h} - mmm$:

Arithmetic classes $mmmP$ and $mmmC$

Decomposition

$mmmP$	$\mathsf{p}mmm$	$\mathsf{p}mcm$	$\mathsf{p}cmm$	$\mathsf{p}ccm$	$\mathsf{v}mmm$
$pmmm$	$^{1}Pmmm$	$^{5}Pmcm$	$^{5}Pcmm$	$^{3}Pccm$	$p\mathsf{v}mmm$
$pmmn$	$^{13}Pmmn$	$^{16}Pmcn$	$^{16}Pcmn$	$^{10}Pccn$	$p\mathsf{v}mmn$
$pbam$	$^{9}Pbam$	$^{16}Pbnm$	$^{16}Pnam$	$^{12}Pnnm$	$p\mathsf{v}bam$
$pban$	$^{4}Pban$	$^{6}Pbnn$	$^{6}Pnan$	$^{2}Pnnn$	$p\mathsf{v}ban$
$pmma$	$^{5}Pmma$	$^{11}Pmca$	$^{9}Pcma$	$^{8}Pcca$	$p\mathsf{v}mma$
$pmmb$	$^{5}Pmmb$	$^{9}Pmcb$	$^{11}Pcmb$	$^{8}Pccb$	$p\mathsf{v}mmb$
$pmam$	$^{5}Pmam$	$^{13}Pmnm$	$^{11}Pcam$	$^{7}Pcnm$	$p\mathsf{v}mam$
$pbmm$	$^{5}Pbmm$	$^{11}Pbcm$	$^{13}Pnmm$	$^{7}Pncm$	$p\mathsf{v}bmm$
$pmaa$	$^{3}Pmaa$	$^{7}Pmna$	$^{8}Pcaa$	$^{4}Pcna$	$p\mathsf{v}maa$
$pbmb$	$^{3}Pbmb$	$^{8}Pbcb$	$^{7}Pnmb$	$^{4}Pncb$	$p\mathsf{v}bmb$
$pmab$	$^{11}Pmab$	$^{16}Pmnb$	$^{15}Pcab$	$^{14}Pcnb$	$p\mathsf{v}mab$
$pbma$	$^{11}Pbma$	$^{15}Pbca$	$^{16}Pnma$	$^{14}Pnca$	$p\mathsf{v}bma$
$pman$	$^{7}Pman$	$^{12}Pmnn$	$^{14}Pcan$	$^{6}Pcnn$	$p\mathsf{v}man$
$pbmn$	$^{7}Pbmn$	$^{14}Pbcn$	$^{12}Pnmn$	$^{6}Pncn$	$p\mathsf{v}bmn$
$pbaa$	$^{8}Pbaa$	$^{14}Pbna$	$^{10}Pnaa$	$^{6}Pnna$	$p\mathsf{v}baa$
$pbab$	$^{8}Pbab$	$^{10}Pbnb$	$^{14}Pnab$	$^{6}Pnnb$	$p\mathsf{v}bab$
$mmmC$					
$cmmm$	$^{19}Cmmm$	$^{17}Cmcm$	$^{17}Ccmm$	$^{20}Cccm$	$c\mathsf{v}mmm$
$cmma$	$^{21}Cmma$	$^{18}Cmca$	$^{18}Ccma$	$^{22}Ccca$	$c\mathsf{v}mma$
$cmmb$	$^{21}Cmmb$	$^{18}Cmcb$	$^{18}Ccmb$	$^{22}Cccb$	$c\mathsf{v}mmb$
$vmmm$	$v\mathsf{p}mmm$	$v\mathsf{p}mcm$	$v\mathsf{p}cmm$	$v\mathsf{p}ccm$	$Vmmm$

Exercise 4: The group $P4_2nmc$ in our system is combined from the rod group $\mathsf{p}4_2/mmc$ and the layer group $p4/nmm$. Systems of nonprimitive translations for these two groups and for the resulting space group are given in the table:

	4_z	2_x	m_z
$\mathsf{p}4_2/mmc$	$\mathbf{c}/2$	$\mathbf{0}$	$\mathbf{0}$
$p4/nmm$	$\mathbf{0}$	$(\mathbf{a}+\mathbf{b})/2$	$(\mathbf{a}+\mathbf{b})/2$
$P4_2/nmc$	$\mathbf{c}/2$	$(\mathbf{a}+\mathbf{b})/2$	$(\mathbf{a}+\mathbf{b})/2$

The nonprimitive translations for point group elements 4_z and 2_x are actually sufficient to determine the location of the groups. We add also nonprimitive translations for the plane m_z. Indeed, an element $\{4_z|\mathbf{c}/2\}$ indicates fourfold screw axis 4_{2z} through the origin, $\{2_x|(\mathbf{a}+\mathbf{b})/2\}$ the screw axis 2_{1x} at a distance $\mathbf{b}/4$ from the origin, which is sufficient to locate the space group $P4_2/nmc$. As an additional information we use the element $\{m_z|(\mathbf{a}+\mathbf{b})/2\}$ which indicates n plane through the origin. Comparing with the diagrams, we obtain that the groups will be denoted in our system by $P4_2/nmc(\mathbf{a}/2+\mathbf{c}/4)$ and $P4_2/nmc[(\mathbf{a}+\mathbf{b})/4]$ for origin choices 1 and 2, respectively.

Exercise 5: (i) If we consider the edges of the diagram as defined by vectors $\mathbf{a}$ (down), $\mathbf{b}$ (to the right) and $\mathbf{c}$ (up) when looking at the diagram so that the group symbol is on its top, then the diagrams represent different groups of the same type which have the translation subgroup $T(\mathbf{a},\mathbf{b},\mathbf{c})$ and point group mmm.

(ii) If we want to interpret the diagrams as the diagrams of the same group from different views, we have to refer each of the groups to a different frame of reference as indicated by symbols of settings.

Exercise 6: Substituting $\varphi(g,\mathbf{s})$ for $\mathbf{u}_G(g)$ in Frobenius congruences we obtain that

$$\mathbf{u}_G(g) + g\mathbf{u}_G(h) - \mathbf{u}_G(gh) = \mathbf{s} - g\mathbf{s} + g\mathbf{s} - gh\mathbf{s} - \mathbf{s} + gh\mathbf{s} \equiv \mathbf{0}.$$

Exercise 7: Since $\mathbf{u}_G(g) \equiv \mathbf{0}$ for every $g \in G$, the group $\mathcal{G}$ contains all elements of the form $\{g|\mathbf{0}\}_P$ which means that it displays the full point symmetry G_P at the origin P. If $\mathbf{u}_G(g) \equiv \varphi(g,\mathbf{s})$, then the group $\mathcal{G}(\mathbf{s})$ contains all elements $\{g|\varphi(g,\mathbf{s})\}_P = \{g|\mathbf{0}\}_{P+\mathbf{s}}$, so that the group displays the full point symmetry $G_{P+\mathbf{s}}$ at the point $P+\mathbf{s}$. It is also easy to see that in this case neither screw axes nor glide planes may exist in $\mathcal{G}$.