

# Isomorphism of lattices of subgroups of the layer and rod groups with sublattices of subgroups of the space groups

Jiri Fuksa\* and Vojtech Kopský

Institute of Physics, Academy of Sciences of the Czech Republic, v.v.i., Na Slovance 2, CZ-182 21 Praha, Czech Republic. Correspondence e-mail: fuksa@fzu.cz

Following a brief overview of current knowledge on lattices of subgroups of the space groups, it is shown that in the case of reducible space groups those lattices contain sublattices which are lattice isomorphic to the lattices of subgroups of layer and rod groups. Both sublattices involve the sublattice consisting of equitranslational subgroups.

© 2011 International Union of Crystallography  
Printed in Singapore – all rights reserved

## 1. Introduction

The bulk of the theory of space-group subgroups has been for a long time based on the well known Hermann theorem (Hermann, 1929), which can be viewed as a special case of the *diamond isomorphism theorem* of algebra (McLane & Birkhoff, 1967). Let us recall its formulation with reference to subgroups of the space groups: ‘A subgroup of a space group is an equiclass subgroup of a certain equitranslational subgroup’. In the early papers in the field, the maximal equitranslational (*translationengleiche*) subgroups and the maximal equiclass (*klassengleiche*) subgroups were listed (Neubüser & Wondratschek, 1966; Boyle & Lawrenson, 1972*a,b*). Ascher contributed to the subject by using an algebraic concept of a lattice (Birkhoff, 1948) for the description of equitranslational subgroups of the space groups (Ascher, 1968). The lattices of subgroups of the point groups were also given by Kopský (1982). The information on maximal isomorphic and non-isomorphic equiclass subgroups of the space groups is provided in the editions of Volume A of *International Tables for Crystallography* (ITC) that have been published since 1983 (Hahn, 1983); analogous information on such subgroups of frieze, layer and rod groups is given in Volume E of ITC (Kopský & Litvin, 2010). These contributions give incomplete information only. Ascher’s lattices show the type of the subgroup but not the exact subgroup and the same concerns Volumes A and E. The first lattices in which the *location* of equitranslational subgroups is specified are a part of the CD ROM published as the electronic supplement to Volume D of ITC (Kopský & Boček, 2003). We note that maximal subgroups of layer and rod groups up to index 4 can be found on the Bilbao Crystallographic Server (<http://www.cryst.ehu.es>). The subgroups are presented by means of transformation matrices there. The concept of the group *location* is consistently used in the specification of standards of the frieze, layer and rod groups as well as in the ‘Scanning tables’ of Volume E. The latest progress of the theory and information on subgroups of the space groups is manifested in

the first edition of Volume A1 of ITC (Wondratschek & Müller, 2004). The volume already takes into account the location of subgroups, and some important lattices are presented there. As an artefact of crystallographic philosophy, Volume A1 describes the *shift of origin* instead of a more appropriate shift of the subgroup itself. In this contribution we consider the correlation of lattices of subgroups of subperiodic groups with lattices of subgroups of the reducible space groups.

### 1.1. Terminological comments

(i) The subgroups of a given group constitute a partially ordered set in which both supremum and infimum with respect to the partial ordering on the set exist for any non-empty finite subset of its elements. In algebra such a set is called a lattice. Unfortunately, English is one of a few European languages in which the term clashes with the crystallographic concept of a vector or a point lattice. The authors of Volume A1 use the term ‘graph’, which does not include all lattice properties; the term ‘tree’ would be completely unacceptable because it denotes a graph without cycles (Ore, 1962).

The table below offers terms in several European languages both for a lattice in a set-theoretical sense and for a lattice as the normal translation subgroup of a space group.

Language	Lattice (set)	Lattice (translations)
français	treillis	réseau
deutsch	Verband	Gitter
español	retículo	red
italiano	reticolo	reticolo
português	reticulado	retículo
но-русски	структура	решётка
česky	svaz	mřížka
polski	krata	sieć

Besides, we also prefer the terms ‘equiclass’ and ‘equitranslational subgroups’ to ‘*klassengleiche*’ and ‘*translationengleiche*’.

(ii) For any two subgroups  $F$  and  $K$  of a group  $G$ , the groups  $\sup\{F, K\}$  and  $\inf\{F, K\}$  are called the group-theoretical union

and the intersection of  $F$  and  $K$ , respectively; only the latter coincides with its set-theoretical analogue,  $\inf\{F, K\} = F \cap K$ . The group-theoretical union of  $F$  and  $K$  contains all finite products of operations belonging to  $F$  or to  $K$ ; yet we prefer to denote it by  $F \cup K$ .

### 2. Beyond the theorem by Hermann

We shall commence this contribution by a formulation of that theorem (Hall, 1959; McLane & Birkhoff, 1967) of which the Hermann theorem is a particular case.

*Theorem 2.1. The diamond isomorphism theorem for groups.* Let  $G$  be a group and  $H$  its normal subgroup. If  $F$  is any other subgroup of the group  $G$ , then  $F \cup H = FH$ , and the factor groups  $FH/H$  and  $F/(F \cap H)$  are isomorphic.

*Notes.* (i) Since  $H$  is normal in  $G$ , then  $hf = fh'$ ,  $h' = f^{-1}hf \in H$ , for any  $f \in F$  and any  $h \in H$ . An element  $f_1h_1f_2h_2 \dots f_sh_s \in F \cup H$  equals  $f_1f_2 \dots f_sh_{1,2,\dots,s} \in FH$  with  $h_{1,2,\dots,s} \in H$ . ( $F \cup H$  contains all elements of the form  $f_1h_1 \dots f_sh_s$  where the operations  $f_1, \dots, f_s \in F$  as well as the operations  $h_1, \dots, h_s \in H$  need not be all distinct.) (ii) The isomorphism  $\varphi : FH/H \rightarrow F/(F \cap H)$  is given by  $fH \rightarrow f(F \cap H)$ ,  $f \in F$ .

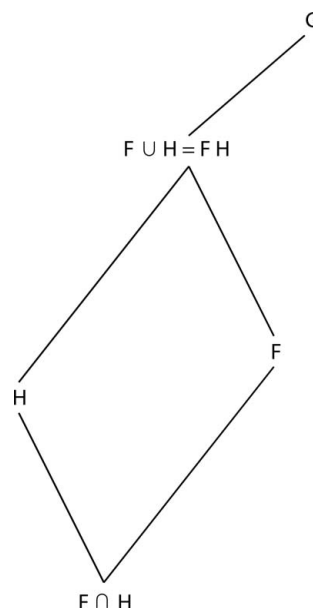
If  $G = \mathcal{G}$  is a space group, then setting  $H = T$  for its maximal translation subgroup, one obtains Hermann's theorem as a corollary. The corollary of the diamond isomorphism theorem is applicable, in general, to Euclidean groups, and in particular to subperiodic groups. The term 'diamond' refers to the shape of the illustrative diagram (see Fig. 1). Some authors speak of the *second isomorphism theorem*.

### 3. Lattice isomorphisms

Let us recall that a *lattice*  $\mathbf{L}$  is a partially ordered set, *i.e.* such a set in which for some elements  $a$  and  $b$  there is defined an ordering relation  $\leq$ : either  $a \leq b$  or  $b \leq a$ . In addition, for any two elements  $a, b$  there exist their least upper bound and their greatest lower bound with respect to  $\leq$ , denoted by  $a \vee b$  and  $a \wedge b$ , respectively. The binary operations of  $\vee$  and  $\wedge$  are called, respectively, *join* and *meet* (Birkhoff, 1948). All elements  $c$  such that  $b \leq c \leq a$  form a sublattice of  $\mathbf{L}$ , called a *quotient*  $\mathbf{L}(a; b)$  (Hall, 1959), or an *interval*  $[a, b]$  (Burris & Sankappanavar, 1981). We prefer the former term to the latter since, in general, such sublattice need not be well ordered.

The set  $\{F, K, \dots\}$  of subgroups of a group  $G$  forms a lattice  $\mathbf{L}(G)$  with respect to the ordinary group-subgroup relation, identical with the set-theoretical inclusion  $\subseteq$ . Analogues of the abstract lattice binary operations of join and meet are the group-theoretical union, denoted by  $\cup$ , and the usual set-theoretical intersection  $\cap$ . Similarly to the definition above, the quotient sublattice  $\mathbf{L}(G; F)$  of  $\mathbf{L}(G)$  consists of all subgroups  $K$  of  $G$  containing  $F$ . Hence, if  $F \subset H \subseteq G$  then  $\mathbf{L}(G; F) \supset \mathbf{L}(G; H)$ .

*Definition 3.1.* Two lattices are said to be lattice isomorphic if there exists a bijection which preserves inclusion relations



**Figure 1** Diagram of 'diamond isomorphism' between factor groups  $FH/H$  and  $F/F \cap H$ , where  $H$  is a normal subgroup of  $G$ .

and/or maps group-theoretical unions and intersections onto group-theoretical unions and intersections, respectively.

*Theorem 3.1. Lattice isomorphism induced by a normal subgroup.* Consider a group  $G$  and its normal subgroup  $H$ . Then the lattice  $\mathbf{L}(\mathcal{H})$  of subgroups of the factor group  $\mathcal{H} = G/H$  is isomorphic to the quotient  $\mathbf{L}(G; H)$  of the lattice  $\mathbf{L}(G)$ .

*Note.* The lattice isomorphism  $\sigma : \mathbf{L}(G; H) \rightarrow \mathbf{L}(\mathcal{H})$  is given by  $K \rightarrow \mathcal{K} = K/H$  for any group  $K, H \subseteq K \subseteq G$ .

*Corollary 3.1.* Suppose  $G$  is a crystallographic point group, and  $\mathcal{G}$  is a space group in the geometric class  $G$ . Let  $\mathbf{L}(G)$  and  $\mathbf{L}(\mathcal{G})$  denote the lattice of subgroups of  $G$  and  $\mathcal{G}$ , respectively. Then, equitranslational subgroups of  $\mathcal{G}$  form a quotient sublattice  $\mathbf{L}(\mathcal{G}; T)$  of  $\mathbf{L}(\mathcal{G})$  which is lattice isomorphic to the lattice  $\mathbf{L}(G)$ .

### 4. Euclidean groups as groups of operators on Euclidean space

Following the cohomology approach of Ascher & Janner (1965, 1968) in its simplified form, we first formulate a theorem which is a good starting point for general considerations of Euclidean groups.

*Theorem 4.1. Fundamental theorem on Euclidean groups.* Every Euclidean group can be expressed by a symbol:

$$\mathcal{G} = \{G, T_G, P, \mathbf{u}_G\},$$

where  $P$  is an origin of the coordinate system,  $G$  is a point group,  $T_G = \mathcal{G} \cap V$  is the maximal ( $G$ -invariant) translation subgroup of  $\mathcal{G}$ ,  $V$  is the Euclidean vector space viewed as the group of all translations, and  $\mathbf{u}_G : G \rightarrow V$  is called the *system*

of nonprimitive translations satisfying so-called Frobenius congruences:

$$\mathbf{w}(g, h) = \mathbf{u}_G(g) + g\mathbf{u}_G(h) - \mathbf{u}_G(gh) = 0 \pmod{T_G}, \quad g, h \in G; \quad (1)$$

$\mathbf{w} : G \times G \rightarrow T_G$  is called a factor system.

The symbol for  $\mathcal{G}$  represents the set of Euclidean operators (isometries) with Seitz symbols  $\{g|\mathbf{t} + \mathbf{u}_G(g)\}_p$  where  $g$  runs through the point group  $G$  and  $\mathbf{t}$  through the translation subgroup  $T_G$ .

Of particular interest is a trivial solution  $\theta_\tau : G \rightarrow V$  to the Frobenius congruences,  $\theta_\tau(g) = \tau - g\tau$ ,  $g \in G$ ,  $\tau \in V$ . Conjugation of individual elements of  $\mathcal{G}$  by a shift  $\{e|\tau\}$  gives one

$$\{e|\tau\}\{g|\mathbf{t} + \mathbf{u}_G(g)\}_p\{e|-\tau\} = \{g|\mathbf{t} + \mathbf{u}_G(g) + \tau - g\tau\}_p.$$

Therefore, if  $\theta_\tau(g) = \tau - g\tau \neq 0 \pmod{T_G}$  for some  $g \in G$ , one obtains another Euclidean group  $\{e|\tau\}\mathcal{G}\{e|-\tau\} = \mathcal{G}(\tau)$ ,

$$\mathcal{G}(\tau) = \{G, T_G, P, \mathbf{u}_G + \theta_\tau\} = \{G, T_G, P + \tau, \mathbf{u}_G\}. \quad (2)$$

The shift  $\tau$  is interpreted in Volume A1 of ITC as the shift of origin. However, it should be interpreted as the shift of the group itself. Indeed, comparison of expressions for the two groups shows that the group  $\mathcal{G}(\tau)$  is described with respect to the origin  $P + \tau$  in the same manner as the group  $\mathcal{G}$  with respect to the origin  $P$  (for example, by the group diagram).

## 5. Presentation of a reducible $G$ -invariant translation group $T_G$

Let us observe that, apart from point groups of the cubic family, all other crystallographic point groups are reducible. Denote by  $\mathbf{a}$ ,  $\mathbf{b}$  and  $\mathbf{c}$  conventional crystallographic basis vectors. In order to avoid ambiguity we stipulate the following: (i) with the rhombohedral space groups the hexagonal basis will be used instead of the rhombohedral one; (ii) with the monoclinic family we will use 'unique axis  $c$ '. Provided that a point group  $G$  belongs to the tetragonal or hexagonal family, the Euclidean vector space  $V$  will be decomposed into a direct sum of two mutually orthogonal  $G$ -invariant subspaces,

$$V = V(\mathbf{a}, \mathbf{b}) \oplus V(\mathbf{c}), \quad (3)$$

where a subspace  $V(\mathbf{a}, \mathbf{b})$  is spanned by the vectors  $\mathbf{a}$  and  $\mathbf{b}$ , and  $V(\mathbf{c})$  is spanned by  $\mathbf{c}$ . In the case where a point group  $G$  belongs to the triclinic, monoclinic or orthorhombic family, one can express the space  $V$  as a direct sum of three  $G$ -invariant subspaces,

$$V = V(\mathbf{a}) \oplus V(\mathbf{b}) \oplus V(\mathbf{c}). \quad (4)$$

In either case, the space  $V$  is *reducible* under the action of  $G$ . One also refers to the point group  $G$  and the respective crystallographic family as reducible.

Consider now a reducible point group  $G$  and the decomposition of  $V$  into a direct sum  $V(\mathbf{a}, \mathbf{b}) \oplus V(\mathbf{c})$  of  $G$ -invariant subspaces (apart from the triclinic case, those subspaces are mutually orthogonal). We introduce projections  $\sigma_1 : V \rightarrow V(\mathbf{a}, \mathbf{b})$  and  $\sigma_2 : V \rightarrow V(\mathbf{c})$  of  $V$  onto its subspaces,  $\tau = \sigma_1(\tau) + \sigma_2(\tau)$  for any  $\tau \in V$ . As intersections of a

$G$ -invariant translation group  $T_G$  with the subspaces of  $V$  one gets  $G$ -invariant direct summands of  $T_G$ : a two-dimensional  $T_{G1} = T_G \cap V(\mathbf{a}, \mathbf{b})$  and a one-dimensional  $T_{G2} = T_G \cap V(\mathbf{c})$ . For either summand there exists a complementary direct summand of  $T_G$  (not necessarily a  $G$ -invariant one), say  $T'_{G2}$  for  $T_{G1}$  and  $T'_{G1}$  for  $T_{G2}$ ,

$$T_G = T_{G1} \oplus T'_{G2} = T'_{G1} \oplus T_{G2} \supseteq T_{G1} \oplus T_{G2},$$

where either  $T'_{G2} \not\subseteq V(\mathbf{c})$  and  $T'_{G1} \not\subseteq V(\mathbf{a}, \mathbf{b})$ , or  $T'_{G2} = T_{G2}$  and  $T'_{G1} = T_{G1}$ . Projecting the group  $T_G$  with  $\sigma_1$  and  $\sigma_2$  into the space  $V$  one obtains  $G$ -invariant discrete translation groups  $\sigma_1(T_G) = T_{G1}^o \supseteq T_{G1}$  and  $\sigma_2(T_G) = T_{G2}^o \supseteq T_{G2}$ . It follows that

$$T_{G1}^o \oplus T_{G2}^o \supseteq T_G \supseteq T_{G1} \oplus T_{G2}. \quad (5)$$

The group  $T_G$  either splits into a direct sum of  $T_{G1}$  and  $T_{G2}$  ( $T_{G1} = T_{G1}$ ,  $T_{G2} = T_{G2}$ ),

$$T_G = T_{G1} \oplus T_{G2}, \quad (6)$$

or equals a subdirect sum of  $G$ -invariant groups  $T_{G1}^o$  and  $T_{G2}^o$ , in which case three factor groups  $T_G/(T_{G1} \oplus T_{G2})$ ,  $T_{G1}^o/T_{G1}$  and  $T_{G2}^o/T_{G2}$  are isomorphic (Hall, 1959). Each factor group is an additive group formed by the respective  $p$  cosets given below.

$$\begin{aligned} T_G &= (T_{G1} \oplus T_{G2}) \cup (\mathbf{d}_1 + (T_{G1} \oplus T_{G2})) \\ &\cup \dots \cup (\mathbf{d}_p + (T_{G1} \oplus T_{G2})) \\ &= (T_{G1} \oplus T_{G2})[\mathbf{0} \cup \mathbf{d}_1 \cup \dots \cup \mathbf{d}_p] \quad (\mathbf{d}_1 = \mathbf{0}), \end{aligned} \quad (7)$$

where  $\mathbf{d}_j + (T_{G1} \oplus T_{G2}) = \{\mathbf{d}_j + \mathbf{t}; \mathbf{t} \in T_{G1} \oplus T_{G2}\}$ ,  $j \in \{1, \dots, p\}$ , and

$$\begin{aligned} \sigma_1(T_G) &= T_{G1}^o = T_{G1} \cup (\mathbf{d}_{12} + T_{G1}) \cup \dots \cup (\mathbf{d}_{1p} + T_{G1}) \\ &= T_{G1}[\mathbf{0} \cup \mathbf{d}_{12} \cup \dots \cup \mathbf{d}_{1p}], \end{aligned}$$

$$\begin{aligned} \sigma_2(T_G) &= T_{G2}^o = T_{G2} \cup (\mathbf{d}_{22} + T_{G2}) \cup \dots \cup (\mathbf{d}_{2p} + T_{G2}) \\ &= T_{G2}[\mathbf{0} \cup \mathbf{d}_{22} \cup \dots \cup \mathbf{d}_{2p}], \end{aligned}$$

with  $\mathbf{d}_{1j} = \sigma_1(\mathbf{d}_j)$ ,  $\mathbf{d}_{2j} = \sigma_2(\mathbf{d}_j)$ ,  $j = 1, \dots, p$ . Cosets add following the common rule, e.g.  $(\mathbf{d}_j + (T_{G1} \oplus T_{G2})) + (\mathbf{d}_k + (T_{G1} \oplus T_{G2})) = \mathbf{d}_l + (T_{G1} \oplus T_{G2})$ ,  $\mathbf{d}_j + \mathbf{d}_k - \mathbf{d}_l \in T_{G1} \oplus T_{G2}$ ,  $j, k = 1, \dots, p$ . The last expressions of the three equations above are symbolic abbreviations which will be used henceforth. The isomorphisms between three factor groups,  $T_G/(T_{G1} \oplus T_{G2}) \leftrightarrow T_{G1}^o/T_{G1} \leftrightarrow T_{G2}^o/T_{G2}$ , are given by

$$\mathbf{d}_j + (T_{G1} \oplus T_{G2}) \leftrightarrow \mathbf{d}_{1j} + T_{G1} \leftrightarrow \mathbf{d}_{2j} + T_{G2}, \quad j = 1, \dots, p. \quad (8)$$

The case of a direct sum [equation (6)] corresponds to primitive lattices [note that the rhombohedral lattice  $R$  is not primitive in terms of the hexagonal basis used (see above)] as well as to a  $C$ -centered orthorhombic lattice, while a subdirect sum [equation (7)] will appear for other centered lattices, in which case the vectors  $\mathbf{d}_j$  represent the centering vectors.

*Definition 5.1.* Consider a reducible point group  $G$  and a  $G$ -invariant translation group  $T_G$ . The presentation of  $T_G$  in the form of a  $G$ -invariant direct sum [equation (6)] is called *decomposition* while the presentation of  $T_G$  in the form of a

**Table 1**

Decomposition of space groups of arithmetic class  $4/mmmP$  by pairs of layer and rod groups.

$4/mmmP$	$\not\wedge 4/mmm$	$\not\wedge 4/mcc$	$\not\wedge 4_2/mmc$	$\not\wedge 4_2/mcm$
$p4/mmm$	$^1P4/mmm$	$^2P4/mcc$	$^9P4_2/mmc$	$^{10}P4_2/mcm$
$p4/nbm$	$^3P4/nbm$	$^4P4/nnc$	$^{11}P4_2/nbc$	$^{12}P4_2/nnm$
$p4/mbm$	$^5P4/mbm$	$^6P4/mnc$	$^{13}P4_2/mbc$	$^{14}P4_2/mnm$
$p4/nmm$	$^7P4/nmm$	$^8P4/ncc$	$^{15}P4_2/nmc$	$^{16}P4_2/ncm$

subdirect sum [equation (7)] of two  $G$ -invariant groups is called *reduction*.

Decomposability and reducibility of discrete translation groups under the action of point groups are properties of the respective Bravais types. All such decompositions and reductions in dimensions 2 and 3 have been considered by Kopský (1993) and Fuksa & Kopský (1993).

### 6. Factorization of reducible space groups by direct summands of $T_G$

Consider a space group  $\mathcal{G} = \{G, T_G, P, \mathbf{u}_G\}$  belonging to a reducible crystallographic family; one refers to  $\mathcal{G}$  as a reducible space group. The  $G$ -invariant direct summands  $T_{G1} = T_G \cap V(\mathbf{a}, \mathbf{b})$  and  $T_{G2} = T_G \cap V(\mathbf{c})$  of  $T_G$  (see §5) will then appear as normal subgroups of  $\mathcal{G}$ . The following theorem identifies the factor groups  $\mathcal{G}/T_{G1}$  and  $\mathcal{G}/T_{G2}$ .

*Theorem 6.1. Factorization theorem.* Suppose  $\mathcal{G} = \{G, T_G, P, \mathbf{u}_G\}$  is a reducible space group. Then the factor group  $\mathcal{G}/T_{G2}$  is isomorphic to a layer group

$$\mathcal{L} = \{G, T_{G1}^o, P, \mathbf{u}_{G1}\},$$

while the factor group  $\mathcal{G}/T_{G1}$  is isomorphic to a rod group

$$\mathcal{R} = \{G, T_{G2}^o, P, \mathbf{u}_{G2}\}.$$

Systems of non-primitive translations  $\mathbf{u}_{G1} : G \rightarrow V(\mathbf{a}, \mathbf{b})$  and  $\mathbf{u}_{G2} : G \rightarrow V(\mathbf{c})$  are given by  $\mathbf{u}_{G1}(g) = \sigma_1(\mathbf{u}_G(g))$  and  $\mathbf{u}_{G2}(g) = \sigma_2(\mathbf{u}_G(g))$  for all  $g \in G$ .

*Proof.* The symbols for  $\mathcal{L}$  and  $\mathcal{R}$  are symbols of Euclidean groups because they satisfy all conditions of the fundamental theorem. In particular, the systems of nonprimitive translations  $\mathbf{u}_{G1} : G \rightarrow V(\mathbf{a}, \mathbf{b})$  and  $\mathbf{u}_{G2} : G \rightarrow V(\mathbf{c})$  satisfy Frobenius congruences modulo  $T_{G1}^o$  and  $T_{G2}^o$ , respectively, since such Frobenius congruences arise as respective projections of the Frobenius congruences for the original system  $\mathbf{u}_G : G \rightarrow V$ . In the case where  $T_G = T_{G1} \oplus T_{G2}$ , the factor groups  $T_G/T_{G2}$  and  $T_G/T_{G1}$  are isomorphic to  $T_{G1}$  and  $T_{G2}$ , respectively; such facts will be indicated by writing  $T_G/T_{G2} \simeq T_{G1}$  and  $T_G/T_{G1} \simeq T_{G2}$ . Then any coset of the factor groups  $\mathcal{G}/T_{G2}$  and  $\mathcal{G}/T_{G1}$  will be of the form  $\{g|\mathbf{t}_1 + \mathbf{u}_G(g)\}_P T_{G2}$ ,  $\mathbf{t}_1 \in T_{G1}$ ,  $g \in G$  and  $\{g|\mathbf{t}_2 + \mathbf{u}_G(g)\}_P T_{G1}$ ,  $\mathbf{t}_2 \in T_{G2}$ ,  $g \in G$ , respectively. The isomorphisms  $\mathcal{G}/T_{G2} \rightarrow \mathcal{L}$  and  $\mathcal{G}/T_{G1} \rightarrow \mathcal{R}$  are as follows:

$$\{g|\mathbf{t}_1 + \mathbf{u}_G(g)\}_P T_{G2} \longrightarrow \{g|\mathbf{t}_1 + \mathbf{u}_{G1}(g)\}_P \in \mathcal{L}, \quad \mathbf{t}_1 \in T_{G1}, g \in G, \tag{9}$$

**Table 2**

Factorization of space groups of arithmetic class  $4/mmmI$ .

$4/mmmI$	$\not\wedge_{1/2} 4/mmm$	$\not\wedge_{1/2} 4_2/mmc$
$\hat{p}4/mmm$	$^{17}I4/mmm$ $^{18}I4/mcm$	—
$\hat{p}4/nbm$	—	$^{19}I4_1/amd$ $^{20}I4_1/acd$

$$\{g|\mathbf{t}_2 + \mathbf{u}_G(g)\}_P T_{G1} \longrightarrow \{g|\mathbf{t}_2 + \mathbf{u}_{G2}(g)\}_P \in \mathcal{R}, \quad \mathbf{t}_2 \in T_{G2}, g \in G. \tag{10}$$

In the case where  $T_G$  is a subdirect sum [equation (7)] it follows that  $T/T_{G2} \simeq T_{G1}[\mathbf{0} \cup \mathbf{d}_2 \cup \dots \cup \mathbf{d}_p]$  and  $T/T_{G1} \simeq T_{G2}[\mathbf{0} \cup \mathbf{d}_2 \cup \dots \cup \mathbf{d}_p]$ . Then the isomorphisms (9) and (10) change to

$$\{g|\mathbf{t}_1 + \sum_{j=2}^p z_j \mathbf{d}_j + \mathbf{u}_G(g)\}_P T_{G2} \longrightarrow \{g|\mathbf{t}_1 + \sum_{j=2}^p z_j \mathbf{d}_{1j} + \mathbf{u}_{G1}(g)\}_P \in \mathcal{L}, \tag{11}$$

$$\{g|\mathbf{t}_2 + \sum_{j=2}^p z_j \mathbf{d}_j + \mathbf{u}_G(g)\}_P T_{G1} \longrightarrow \{g|\mathbf{t}_2 + \sum_{j=2}^p z_j \mathbf{d}_{2j} + \mathbf{u}_{G2}(g)\}_P \in \mathcal{R}, \tag{12}$$

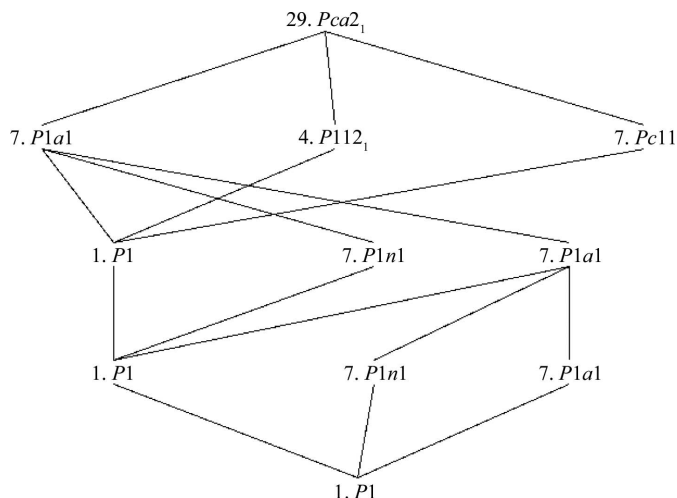
where  $\mathbf{t}_1 \in T_{G1}$ ,  $\mathbf{t}_2 \in T_{G2}$ ,  $z_j \in \{0, 1\}$ ,  $\mathbf{d}_j = \mathbf{d}_{1j} + \mathbf{d}_{2j} \in T_G$ ,  $\mathbf{d}_{1j} \in T_{G1}^o$ ,  $\mathbf{d}_{2j} \in T_{G2}^o$ ,  $j = 2, \dots, p$ , and  $g \in G$ . Using Theorem 3.1, one directly obtains the following corollary.

*Corollary 6.1. Lattices of subgroups of rod and layer groups as quotients of reducible space groups.* The lattice  $\mathbf{L}(\mathcal{L})$  of subgroups of the layer group  $\mathcal{L}$  is lattice isomorphic to the quotient  $\mathbf{L}(\mathcal{G}; T_{G2})$  of the lattice  $\mathbf{L}(\mathcal{G})$  of subgroups of the reducible space group  $\mathcal{G}$ , and the lattice  $\mathbf{L}(\mathcal{R})$  of subgroups of the rod group  $\mathcal{R}$  is lattice isomorphic to the quotient  $\mathbf{L}(\mathcal{G}; T_{G1})$ .

### 7. Illustrative examples

The factorization theorem assigns to a reducible space group  $\mathcal{G} \sim (G, T_G)$  a pair  $(\mathcal{L}, \mathcal{R})$  composed of a layer group  $\mathcal{L} \sim (G, T_{G1}^o)$  and a rod group  $\mathcal{R} \sim (G, T_{G2}^o)$  (Kopský, 1993; Fuksa & Kopský, 1993). In the case when  $T_G$  is a direct sum [equation (6)], the right-hand sides of (9) and (10) imply that the group  $\mathcal{G}$  can be viewed as a result of the *Schreier multiplication* (Kopský, 2001)  $\mathcal{L} \diamond \mathcal{R}$  of the two subperiodic groups (*cf.* Table 1). Otherwise [*cf.* the right-hand sides of equations (11), (12)], the same pair may correspond to two space groups (Fuksa & Kopský, 1993; for an excerpt see Table 2). In both the tables space groups are denoted by Hermann–Mauguin symbols equipped with a Schoenflies superscript at the upper left.

As the first example we present the decomposition table for an arithmetic class  $4/mmmP$  (*cf.* Table 1). In the  $j$ th column heading we give a rod group  $\mathcal{R}^j$ ,  $j \in \{1, 2, 3, 4\}$ , of the class  $4/mmmP$ , while in the  $i$ th row heading we give a layer group  $\mathcal{L}^i$ ,  $i \in \{1, 2, 3, 4\}$ , of the class  $4/mmmP$ . At the intersection of the  $i$ th row with the  $j$ th column there is a space group

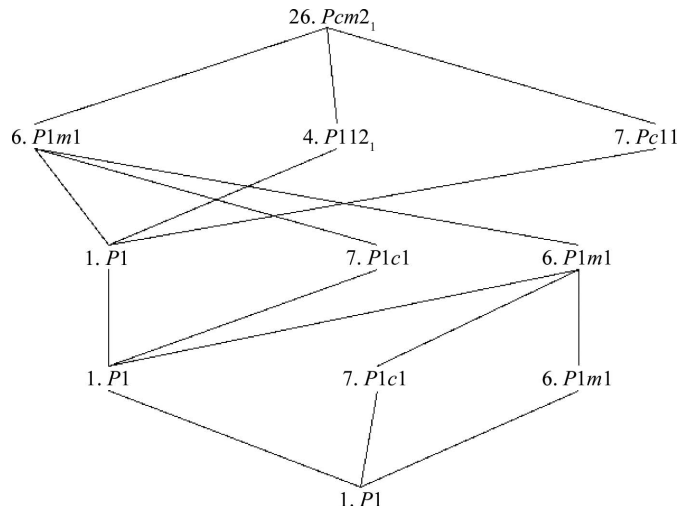


**Figure 2**  
Quotient sublattice  $\mathbf{L}(Pca2_1; T(\mathbf{a}, \mathbf{b}, 4\mathbf{c})) \simeq \mathbf{L}(\bar{1}cm2_1; T(4\mathbf{c}))$ .

$\mathcal{G}^{(i,j)}$ ,  $i, j = 1, 2, 3, 4$ ,  $\mathcal{G}^{(i,j)} \simeq \mathcal{L}^i \diamond \mathcal{R}^j$ . Underlined in Table 1 is an example of the space group  ${}^4P4/nnc \simeq p4/nbm \diamond \bar{1}4/mcc$  where  $\mathbf{L}({}^4P4/nnc; T(\mathbf{c})) \simeq \mathbf{L}(p4/nbm)$  and  $\mathbf{L}({}^4P4/nnc; T(\mathbf{a}, \mathbf{b})) \simeq \mathbf{L}(\bar{1}4/mcc)$ . Each row and each column of Table 1 implies four lattice isomorphisms, e.g. the third row yields  $\mathbf{L}(p4/nbm) \simeq \mathbf{L}({}^5P4/nbm; T(\mathbf{c})) \simeq \dots \simeq \mathbf{L}({}^{14}P4_2/nmm; T(\mathbf{c}))$  while the fourth column reads  $\mathbf{L}(\bar{1}4_2/mmc) \simeq \mathbf{L}({}^{10}P4_2/mcm; T(\mathbf{a}, \mathbf{b})) \simeq \dots \simeq \mathbf{L}({}^{16}P4_2/ncm; T(\mathbf{a}, \mathbf{b}))$ .

The beauty of such a system is, unfortunately, marred by the choice of origins of the space groups. The exact form of the tables should contain respective shifts of space groups to correlate them with the choice of the origins of layer and rod groups.

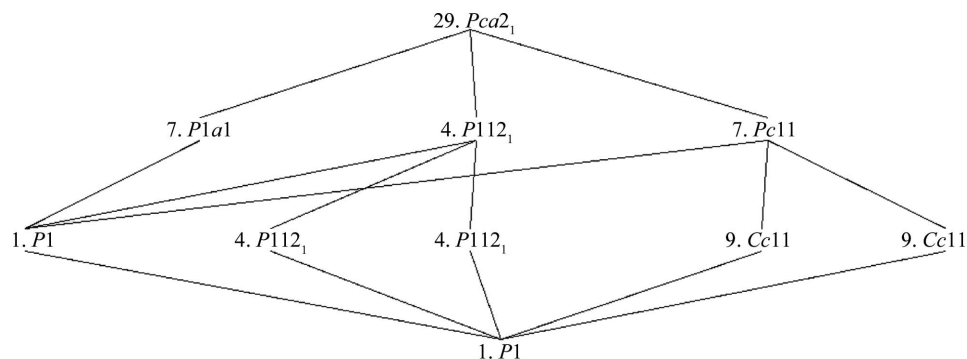
As the second example we give factorization of an arithmetic class  $4/mmmI$  (cf. Table 2) where  $p = 2$ . Vectors  $\mathbf{a}, \mathbf{b}, \mathbf{d}_2 = (\mathbf{a} + \mathbf{b} + \mathbf{c})/2$  form a primitive basis for a volume centered tetragonal lattice  $T_G = T_I$ . As direct summands complementary to  $T_{G1} = T(\mathbf{a}, \mathbf{b})$  and  $T_{G2} = T(\mathbf{c})$  one can take e.g.  $T'_{G2} = T(\mathbf{d}_2)$  and  $T'_{G1} = T(\mathbf{a}, \mathbf{d}_2)$ , respectively. By  $\hat{p}$  we denote the two-dimensional primitive square translation group  $T_{G1} = T(\mathbf{d}_{12} = (\mathbf{a} + \mathbf{b})/2, (-\mathbf{a} + \mathbf{b})/2)$ , and by  $\bar{1}_{1/2}$  the one-dimensional group  $T_{G2} = T(\mathbf{d}_{22} = \mathbf{c}/2)$ . Like Table 1, rod groups of the class  $4/mmm\bar{1}$  are given in the column headings,



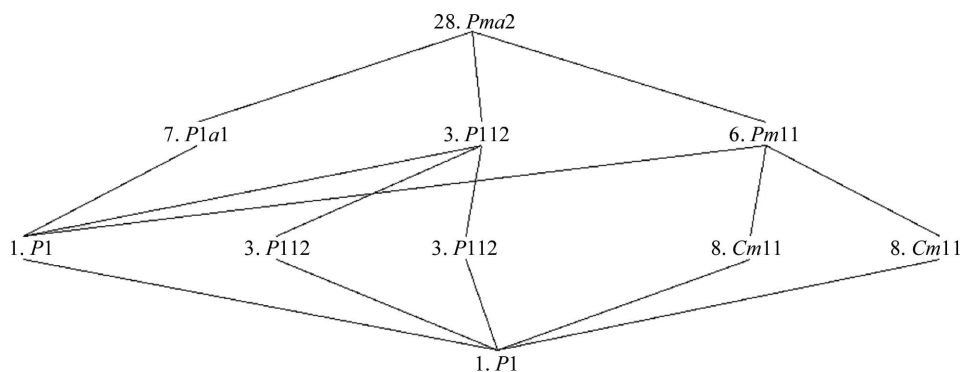
**Figure 3**  
Quotient sublattice  $\mathbf{L}(Pcm2_1; T(\mathbf{a}, \mathbf{b}, 4\mathbf{c})) \simeq \mathbf{L}(\bar{1}cm2_1; T(4\mathbf{c}))$ .

while layer groups of the class  $4/mmm\bar{p}$  are given in the row headings. In contrast to Table 1, some table entries are empty. Table 2 implies  $\mathbf{L}(\hat{p}4/mmm) \simeq \mathbf{L}({}^{17}I4/mmm; T(\mathbf{c})) \simeq \mathbf{L}({}^{18}I4/mcm; T(\mathbf{c}))$  or  $\mathbf{L}(\bar{1}_{1/2}4_2/mmc) \simeq \mathbf{L}({}^{19}I4_1/amd; T(\mathbf{a}, \mathbf{b})) \simeq \mathbf{L}({}^{20}I4_1/acd; T(\mathbf{a}, \mathbf{b}))$ .

As the third example we consider a space group  $Pca2_1 \simeq pma2 \diamond \bar{1}cm2_1$ . The same layer or rod group appears for space groups  $Pma2 \simeq pma2 \diamond \bar{1}mm2$  and  $Pcm2_1 \simeq pmm2 \diamond \bar{1}cm2_1$ . Isomorphisms of the infinite quotients of  $\mathbf{L}(Pca2_1)$  and  $\mathbf{L}(Pcm2_1)$  with the lattice  $\mathbf{L}(\bar{1}cm2_1)$ ,  $\mathbf{L}(Pca2_1; T(\mathbf{a}, \mathbf{b})) \simeq \mathbf{L}(Pcm2_1; T(\mathbf{a}, \mathbf{b})) \simeq \mathbf{L}(\bar{1}cm2_1)$ , are illustrated on finite quotient sublattices  $\mathbf{L}(Pca2_1; T(\mathbf{a}, \mathbf{b}, 4\mathbf{c})) \simeq \mathbf{L}(Pcm2_1; T(\mathbf{a}, \mathbf{b}, 4\mathbf{c})) \simeq \mathbf{L}(\bar{1}cm2_1; T(4\mathbf{c}))$  (see Figs. 2 and 3). The three triclinic groups  $1. P1$  shown there (from above) are  $T(\mathbf{a}, \mathbf{b}, \mathbf{c})$ ,  $T(\mathbf{a}, \mathbf{b}, 2\mathbf{c})$  and  $T(\mathbf{a}, \mathbf{b}, 4\mathbf{c})$ . One gets the quotient  $\mathbf{L}(\bar{1}cm2_1; T(4\mathbf{c}))$  from Fig. 3 just by substituting  $T(\mathbf{c})$ ,  $T(2\mathbf{c})$ ,  $T(4\mathbf{c})$  for  $T(\mathbf{a}, \mathbf{b}, \mathbf{c})$ ,  $T(\mathbf{a}, \mathbf{b}, 2\mathbf{c})$ ,  $T(\mathbf{a}, \mathbf{b}, 4\mathbf{c})$ , respectively, and  $\bar{1}$  for  $P$ . Isomorphisms of the infinite quotients of  $\mathbf{L}(Pca2_1)$  and  $\mathbf{L}(Pma2)$  with the lattice  $\mathbf{L}(pma2)$ ,  $\mathbf{L}(Pca2_1; T(\mathbf{c})) \simeq \mathbf{L}(Pma2; T(\mathbf{c})) \simeq \mathbf{L}(pma2)$ , are illustrated on finite quotients  $\mathbf{L}(Pca2_1; T(\mathbf{a} + \mathbf{b}, -\mathbf{a} + \mathbf{b}, \mathbf{c})) \simeq \mathbf{L}(Pma2; T(\mathbf{a} + \mathbf{b}, -\mathbf{a} + \mathbf{b}, \mathbf{c})) \simeq \mathbf{L}(pma2; T(\mathbf{a} + \mathbf{b}, -\mathbf{a} + \mathbf{b}))$  (see Figs. 4 and 5). The two triclinic groups  $1. P1$  shown there (from above) are  $T(\mathbf{a}, \mathbf{b}, \mathbf{c})$ ,  $T(\mathbf{a} + \mathbf{b}, -\mathbf{a} + \mathbf{b}, \mathbf{c})$ . The quotient  $\mathbf{L}(pma2;$



**Figure 4**  
Quotient sublattice  $\mathbf{L}(Pca2_1; T(\mathbf{a} + \mathbf{b}, -\mathbf{a} + \mathbf{b}, \mathbf{c})) \simeq \mathbf{L}(pma2; T(\mathbf{a} + \mathbf{b}, -\mathbf{a} + \mathbf{b}))$ .



**Figure 5**  
 Quotient sublattice  $\mathbf{L}(Pma2; T(\mathbf{a} + \mathbf{b}, -\mathbf{a} + \mathbf{b}, \mathbf{c})) \simeq \mathbf{L}(pma2; T(\mathbf{a} + \mathbf{b}, -\mathbf{a} + \mathbf{b}))$ .

$T(\mathbf{a} + \mathbf{b}, -\mathbf{a} + \mathbf{b})$  is obtained from Fig. 5 simply by replacing  $T(\mathbf{a}, \mathbf{b}, \mathbf{c})$ ,  $T(\mathbf{a} + \mathbf{b}, -\mathbf{a} + \mathbf{b}, \mathbf{c})$  in the corresponding order, with  $T(\mathbf{a}, \mathbf{b})$ ,  $T(\mathbf{a} + \mathbf{b}, -\mathbf{a} + \mathbf{b})$ , and  $P, C$  with  $p, c$ , respectively. Note that in each pair of translationally equivalent subgroups appearing on both Figs. 4 and 5, the one on the right is shifted with respect to that on the left [according to equation (2)] by  $-\mathbf{a}/2$ .

### 8. Concluding remarks

It is shown that for any reducible space group  $\mathcal{G}$  the lattice  $\mathbf{L}(\mathcal{G})$  of its subgroups contains a copy of the lattice  $\mathbf{L}(\mathcal{R})$  of subgroups of a rod group  $\mathcal{R}$  as well as a copy of the lattice  $\mathbf{L}(\mathcal{L})$  of subgroups of a layer group  $\mathcal{L}$ . Those relationships can facilitate the determination of space-group subgroups, or can serve as an additional check of the subgroups found.

The work was done within the project AVOZ 10100520 of the Academy of Sciences of the Czech Republic. Financial support by the Grant Agency of the AS CR under project No. IAA100100918 is acknowledged.

### References

Ascher, E. (1968). *Lattices of Equi-translation Subgroups of the Space Groups*. Switzerland: Battelle Institute.

Ascher, E. & Janner, A. (1965). *Helv. Phys. Acta*, **38**, 551–572.  
 Ascher, E. & Janner, A. (1968). *Commun. Math. Phys.* **11**, 138–167.  
 Birkhoff, G. (1948). *Lattice Theory* (Colloq. Publ. XXV). New York: American Mathematical Society.  
 Boyle, L. L. & Lawrenson, J. E. (1972a). *Acta Cryst.* **A28**, 485–489.  
 Boyle, L. L. & Lawrenson, J. E. (1972b). *Acta Cryst.* **A28**, 489–493.  
 Burris, S. N. & Sankappanavar, H. P. (1981). *A Course in Universal Algebra*. New York: Springer-Verlag.  
 Fuksa, J. & Kopský, V. (1993). *Acta Cryst.* **A49**, 280–287.  
 Hahn, Th. (1983). Editor. *International Tables for Crystallography*, Vol. A. Dordrecht: D. Reidel.  
 Hall, M. (1959). *Theory of Groups*. New York: McMillan.  
 Hermann, C. (1929). *Z. Kristallogr.* **69**, 533–555.  
 Kopský, V. (1982). *Group Lattices, Subduction of Bases and Fine Domain Structures for the Magnetic Crystal Point Groups*. Prague: Academia.  
 Kopský, V. (1993). *Acta Cryst.* **A49**, 269–280.  
 Kopský, V. (2001). *Advances in Structure Analysis*, edited by R. Kužel & J. Hašek, pp. 334–353. Prague: Czech and Slovak Crystallographic Association.  
 Kopský, V. & Boček, P. (2003). CD-ROM supplement to *International Tables for Crystallography*, Vol. D, edited by A. Authier. Dordrecht: Kluwer.  
 Kopský, V. & Litvin, D. B. (2010). Editors. *International Tables for Crystallography*, Vol. E. Chichester: Wiley.  
 McLane, S. & Birkhoff, G. (1967). *Algebra*. New York: McMillan.  
 Neubüser, J. & Wondratschek, H. (1966). *Krist. Tech.* **1**, 529–543.  
 Ore, O. (1962). *Theory of Graphs* (Colloq. Publ. XXXVIII). New York: American Mathematical Society.  
 Wondratschek, H. & Müller, U. (2004). Editors. *International Tables for Crystallography*, Vol. A1. Heidelberg: Springer.