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Subperiodic groups isomorphic to factor groups of reducible space groups¹

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A relationship exists between factor groups of space groups and subperiodic groups. This relationship, an isomorphism between factor groups of reducible space groups and subperiodic groups, can be used in the derivation of higher-dimensional space groups, of lattices of space groups, and of irreducible representations of space groups. Tables of the layer and rod subperiodic groups isomorphic to factor groups of reducible space groups are explicitly given. The manifestation of this relationship, in terms of the symmetry diagrams of space groups and subperiodic groups, is also discussed.

1. Introduction

The group-subgroup relationship between the three-dimensional space groups and their subperiodic subgroups, i.e. layer groups and rod groups, has been set out in Volume E of International Tables for Crystallography (2000) [abbreviated here as ITCE (2000)]. An additional relationship between space groups and subperiodic groups is generally less well known although one of its manifestations, the fact that for each layer group there exists a space group with the same symmetry and general-position diagram, has been known for quite a while (Cochran, 1952; Lonsdale, personal communication). The algebraic explanation for this was given by Kopský (1989a, 1993) in parallel with the explanation of another fact, that the diagrams of rod groups can also be found within diagrams of certain space groups. The relationship is an isomorphism, that subperiodic groups are isomorphic to factor groups of reducible space groups. Reducibility of space groups, whose definition is given in §2, was introduced and its consequences, among which are the above-mentioned relationships, are described in a dimension-independent manner by the separation theorem and separation diagram (Kopský, 1986). The same isomorphism relationship occurs between factor groups of plane groups (two-dimensional space groups) and frieze groups (two-dimensional groups with one-dimensional translations), and between factor groups of layer groups and frieze groups (Litvin & Kopský, 1987). This relationship is set forth in §3 and in §4 are given tables of the layer and rod groups isomorphic to factor groups of reducible space groups. In §5, the relationship between the symmetry diagrams of reducible space groups and the symmetry diagrams of layer and rod groups is discussed.

This isomorphism can be and is used in additional crystal-lographic procedures. These include the derivation of higher-dimensional space or subperiodic groups (Jarratt, 1980; Kopský, 1988a), of lattices of normal subgroups of space groups (Kopský, 1987), and of irreducible representations of space groups (Kopský, 1988b).

2. Reducible space groups

A reducible space group **G** is defined by the following property (Kopský, 1989*a*,*b*, 1993; Fuksa & Kopský, 1993):

There exist at least one pair of translational subgroups of the translational subgroup T of G, the first one-dimensional and the second two-dimensional, denoted, respectively, by T_{G1} and T_{G2} , where:

- (P1) each subgroup \mathbf{T}_{G1} and \mathbf{T}_{G2} is individually invariant under all rotational parts of the symmetry operations of \mathbf{G} ;
- (P2) each subgroup \mathbf{T}_{G1} and \mathbf{T}_{G2} is maximal in the sense that all translations of \mathbf{T} in the plane of the translations of \mathbf{T}_{G2} are contained in \mathbf{T}_{G2} , and all translations of \mathbf{T} along the direction of the translations of \mathbf{T}_{G1} are contained in \mathbf{T}_{G1} ;

(P3) either

$$\mathbf{T} = \mathbf{T}_{G1} \oplus \mathbf{T}_{G2} \tag{1}$$

or

$$\mathbf{T} = \mathbf{T}_{G1} \oplus \mathbf{T}_{G2}[\mathbf{t}_1 + \mathbf{t}_2 + \ldots + \mathbf{t}_p], \tag{2}$$

where $\mathbf{t}_1 = \mathbf{0} \equiv 0, 0, 0$ and p is a finite integer.

In the first case [equation (1)], the symbol \oplus denotes that each translation of the translational subgroup \mathbf{T} of \mathbf{G} is the sum of a translation of the subgroup \mathbf{T}_{G1} and a translation of the subgroup \mathbf{T}_{G2} . In the second case [equation (2)], the translations of the groups \mathbf{T}_{G1} and \mathbf{T}_{G2} generate only a subgroup of \mathbf{T} . Each translation of the translational subgroup \mathbf{T} of \mathbf{G} is the sum of a translation of the subgroup \mathbf{T}_{G1} , a

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translation of the subgroup \mathbf{T}_{G2} , and a translation from among the set of translations \mathbf{t}_i , i = 1, 2, ..., p.

 T_{G1} and T_{G2} are referred to as *partial translational subgroups* that are *maximal G-invariant* translational proper subgroups of T, G-invariant because of property P1, *maximal* because of property P2 and *partial* because of property P3. The case where equation (1) is satisfied is referred to as a Z-decomposition. This is a special case of equation (2). The more general case [equation (2)] is referred to as a Z-reduction. All space groups except the cubic space groups are reducible space groups.

For a reducible space group, the pairs of partial translational subgroups \mathbf{T}_{G1} and \mathbf{T}_{G2} satisfying equations (1) or (2) depend only on the space group's Bravais-lattice type. In Table 1,² we have tabulated, for each crystallographic system of reducible space groups, the pairs of partial translational subgroups \mathbf{T}_{G1} and \mathbf{T}_{G2} satisfying (1) or (2). For each crystallographic system, we tabulate all Bravais-lattice types listed in Volume A of *International Tables for Crystallography* (1983) [abbreviated here as *ITCA* (1983)].

Each subtable of Table 1 is headed by the name of the corresponding crystallographic system. In the first column is the symbol of the Bravais type, and the second and third columns list \mathbf{T}_{G2} and \mathbf{T}_{G1} , respectively. In each case, we assume that the conventional lattice basis vectors are denoted by \mathbf{a} , \mathbf{b} and \mathbf{c} . We denote \mathbf{T}_{G2} by $\mathbf{T}(\mathbf{n}, \mathbf{m})$, where \mathbf{n} and \mathbf{m} are a pair of generating lattice vectors of \mathbf{T}_{G2} , and \mathbf{T}_{G1} by $\mathbf{T}(\mathbf{q})$, where \mathbf{q} is a generating lattice vector of \mathbf{T}_{G1} . In the fourth column, we write the symbol o or i to denote whether the direction of the translations of \mathbf{T}_{G1} is *orthogonal* or *inclined* with respect to the plane containing the translations of \mathbf{T}_{G2} . In the orthorhombic, tetragonal and hexagonal systems, this column is not given as all cases are orthogonal. The next column gives the corresponding form of the appropriate equation, either (1) or (2).

The final two columns list, respectively, the symbol p or c for a two-dimensional translational group and the symbol p for a one-dimensional translational group. The two-dimensional translational group is determined by projecting the translations of \mathbf{T} along the direction of the translations of \mathbf{T}_{G1} onto the plane of the translations of \mathbf{T}_{G2} . The one-dimensional translational group is determined by projecting the translations of \mathbf{T} along the plane of the translations of \mathbf{T}_{G2} onto the direction of the translations of \mathbf{T}_{G1} . Subindices are provided to uniquely specify these translational groups with respect to the lattice vectors of the translational group \mathbf{T} . These one- and two-dimensional translational groups are (see §3) the translational subgroups of the rod and layer groups isomorphic to factor groups of the reducible space groups.

For example, in the orthorhombic system, one line of the subtable corresponding to the Bravais lattice type I reads:

I
$$\mathbf{T}(\mathbf{a}, \mathbf{b}) \mathbf{T}(\mathbf{c}) \mathbf{T}(\mathbf{a}, \mathbf{b}) \oplus \mathbf{T}(\mathbf{c})[\mathbf{0} + \frac{1}{2}(\mathbf{a} + \mathbf{b} + \mathbf{c})] c_{\mathbf{a}, \mathbf{b}} p_{\mathbf{c}/2}.$$

Here, $\mathbf{T}_{G2} = \mathbf{T}(\mathbf{a}, \mathbf{b})$, $\mathbf{T}_{G1} = \mathbf{T}(\mathbf{c})$ and this pair of translational subgroups satisfies equation (2) with p = 2, $\mathbf{t}_1 = \mathbf{0} \equiv 0$, 0, 0 and $\mathbf{t}_2 = \frac{1}{2}(\mathbf{a} + \mathbf{b} + \mathbf{c}) \equiv \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$. Projecting all translations of a lattice belonging to type I onto the ab plane gives rise to the two-dimensional centered translational group $\langle \frac{1}{2}, -\frac{1}{2}, 0; \frac{1}{2}, \frac{1}{2}, 0 \rangle$ denoted by $\mathbf{c}_{a,b}$. Projecting all translations of this I lattice type onto the c direction gives rise to the one-dimensional translational group $\langle 0, 0, \frac{1}{2} \rangle$ denoted by $p_{\mathbf{c}/2}$.

3. Factor groups of reducible space groups

Let G be a reducible space group and T_{G1} and T_{G2} be partial translational subgroups that satisfy either equation (1) or equation (2). The factor groups of G with respect to these partial translational subgroups have the structure of subperiodic groups (Kopský, 1986, 1993; Kopský & Litvin, 1987; Fuksa & Kopský, 1993). The factor group G/T_{G1} has the structure of a layer group of a specific type and the factor group G/T_{G2} has the structure of a rod group of a specific type.

For the purpose of tabulation of the layer and rod groups isomorphic to the factor groups $\mathbf{G}/\mathbf{T}_{G1}$ and $\mathbf{G}/\mathbf{T}_{G2}$, we first select a single space group \mathbf{G} from each space-group type. This is the space group, in a coordinate system $(\mathbf{0}; \mathbf{a}, \mathbf{b}, \mathbf{c})$, given as the first setting in ITCA (1983) on the page headed by the symbol for that space-group type. If different origins or cell choices are listed in ITCA (1983), separate tabulations are given for each. For a given $\mathbf{G}, \mathbf{T}_{G1}$ and \mathbf{T}_{G2} , we tabulate a single layer group of the type isomorphic to $\mathbf{G}/\mathbf{T}_{G1}$ and a single rod group of the type isomorphic to $\mathbf{G}/\mathbf{T}_{G2}$. The layer group is the sectional layer group (see ITCE, 2000) of that plane passing through the origin of the coordinate system of the space group that is invariant under the translations of \mathbf{T}_{G2} . The rod group is the penetrating rod group of that line passing through the origin invariant under the translations of \mathbf{T}_{G1} .

Consequently, to each reducible space group we associate a pair of subperiodic groups, a layer group isomorphic to the factor group $\mathbf{G}/\mathbf{T}_{G1}$ and a rod group isomorphic to the factor group $\mathbf{G}/\mathbf{T}_{G2}$. A reducible space group may have more than a single pair of partial translational subgroups \mathbf{T}_{G1} and \mathbf{T}_{G2} that satisfy either (1) or (2). Therefore, a reducible space group may have associated with it more than a single layer and rod-group pair.

To determine a rod group isomorphic to the factor group $\mathbf{G}/\mathbf{T}_{G2}$, one lists a set of coset representatives G_i of the cosets $G_i\mathbf{T}_{G2}$ in the coset decomposition of \mathbf{G} with respect to \mathbf{T}_{G2} . In each coset representative $G_i = (R_i|T_i)$, $T_i = T_{i1} + T_{i2}$, where T_{i1} is the component of the translation T_i in the direction of the translations of \mathbf{T}_{G1} and T_{i2} is the component of the translation G_i in the plane of the translations of \mathbf{T}_{G2} . For each element $G_i = (R_i|T_i)$, one defines the element $G_{i1} = (R_i|T_{i1})$. The set of elements G_{i1} constitutes a rod group isomorphic to the factor group $\mathbf{G}/\mathbf{T}_{G2}$. While the choice of coset representative G_i in the coset decomposition of \mathbf{G} with respect to \mathbf{T} is not unique, the type of rod group so derived is unique.

To determine a layer group isomorphic to the factor group $\mathbf{G}/\mathbf{T}_{G1}$, one lists a set of coset representatives G_i of the cosets

² Complete Table 1 and Table 2 referred to in this paper are available from the IUCr electronic archives (Reference: DR0001). Services for accessing these data are described at the back of the journal.

 $G_i\mathbf{T}_{G1}$ in the coset decomposition of \mathbf{G} with respect to \mathbf{T}_{G1} . For each element $G_i = (R_i|T_i)$, one defines the element $G_{i2} = (R_i|T_{i2})$. The set of elements G_{i2} constitutes a layer group isomorphic to the factor group $\mathbf{G}/\mathbf{T}_{G1}$.

4. Tables of layer and rod groups isomorphic to factor groups of reducible space groups

In Table 2, we have tabulated the layer and rod groups isomorphic to factor groups of all reducible space groups. The format of the table is as follows:

The table is subdivided into five subtables listing the space groups according to their Bravais lattice type. These five subtables have the headings Triclinic system, Monoclinic system, Orthorhombic system, Tetragonal system and Hexagonal system.

In the first column of each subtable, we list the number and symbol of a reducible space group **G**. The numbering of the space group is according to the space-group type and follows the numbering as given in ITCA (1983). In general, we choose one space group from each type of reducible space group. For some types of reducible space group, more than a single space group of that type is considered. These cases correspond to those cases in ITCA (1983) where there are two origin choices listed for a space-group type, e.g. the space-group type P4/n (No. 85, C_{4h}^3), when two unique axes are listed for a space-group type, e.g. $P2_1/m$ (No. 11, C_{2h}^2), and when trios of cell choices are listed for a space-group type, e.g. C2/m (No. 12, C_{2h}^3).

Origin choices are denoted in parentheses immediately following the space-group symbol with the acronyms OC1 and OC2 denoting *origin choice 1* and *origin choice 2*, respectively, e.g. P4/n(OC1) and P4/n(OC2). The two unique axes are denoted by the acronyms UAb and UAc denoting respectively unique axis b and unique axis c. The cell choices are denoted by the acronyms CH1, CH2 and CH3, denoting *cell choice 1*, *cell choice 2* and *cell choice 3*, respectively. In monoclinic cases, a second symbol for the space group is given in parentheses specifying a unique symbol for the case considered. For example,

denotes the space group C2/m with unique axis c, cell choice 3, and which is denoted by B112/m.

For the rhombohedral space groups, e.g. R3 (No. 146, C_3^4), two coordinate systems are used: hexagonal axes, denoted by H and rhombohedral axes, denoted by R. Consequently, for each of these space groups there are two sets of entries in Table 2. These two sets are distinguished by the letter H or R given in parentheses after the space-group symbol, e.g. R3 (H) and R3 (R).

The partial translational subgroups \mathbf{T}_{G2} and \mathbf{T}_{G1} are given, respectively, in the second and third columns of Table 2 for space groups of the triclinic, monoclinic and orthorhombic systems. The subgroup \mathbf{T}_{G2} is given in the format $\mathbf{T}(\mathbf{n}, \mathbf{m})$ and

 T_{G1} in the format T(q). The translations \mathbf{n} , \mathbf{m} and \mathbf{q} are given in terms of the conventional basis \mathbf{a} , \mathbf{b} and \mathbf{c} of the space group \mathbf{G} . For space groups of the tetragonal and hexagonal systems, where the partial translational subgroups are the same for all space groups in each system, the subgroups T_{G2} and T_{G1} are listed to the right of the system heading. For example: (i) for the space group No. 21 C222, we have $T_{G2} = T(\frac{1}{2}(\mathbf{a} - \mathbf{b}), \frac{1}{2}(\mathbf{a} + \mathbf{b}))$ and $T_{G1} = T(\mathbf{c})$; and (ii) for all space groups of the tetragonal system, $T_{G2} = T(\mathbf{a}, \mathbf{b})$ and $T_{G1} = T(\mathbf{c})$. If more than a single pair of subgroups T_{G2} and T_{G1} are associated with the same space group, they are given in consecutive rows of Table 2 adjacent to the symbol of the space group \mathbf{G} .

In the following three columns, the layer group isomorphic to the factor group $\mathbf{G}/\mathbf{T}_{G1}$, determined by the procedure given in §3, is specified. In the first of the three columns, the layer-group type is given. If in the coordinate system of the space group \mathbf{G} the translations and symmetry operations of the layer group are identical with the translations and symmetry operations of the layer group listed in *ITCE* (2000) on the page headed by the layer-group-type symbol given in the first column, then the basis vectors \mathbf{a} , \mathbf{b} , \mathbf{c} are given in the second column. \mathbf{a} , \mathbf{b} and \mathbf{c} are then the basis vectors of the conventional coordinate system of the space group and of the layer group, with the first two basis vectors generating the translational subgroup of the layer group. The third column is then left blank.

In the coordinate system of the space group G, the translations and symmetry operations of the layer group may not be identical with the translations and symmetry operations of the layer group listed in *ITCE* (2000) on the page headed by the layer-group-type symbol given in the first column. In such a case, a change in the basis vectors and/or a shift in origin is required to make them identical. If required, a new set of basis vectors for the layer group is given in the second column in terms of the basis vectors of the space group's conventional coordinate system. If required, a shift vector is given in the third column. For example: For the space group $P2_12_12_1$ (No. 19, D_2^4), one finds in Table 2:

19)
$$P2_12_12_1$$
 T(b, c) T(a) $p2_12_12$ **b, c, a b**/4.

The layer group isomorphic to $\mathbf{G}/\mathbf{T}_{G1}$ has in the coordinate system of the space group \mathbf{G} the translational subgroup (0, 1, 0; 0, 0, 1) and the symmetry operations, given in both Seitz notation and the notation of ITCA (1983):

$$(E|0, 0, 0) = 1$$

$$(2z|0, 0, \frac{1}{2}) = 2(0, 0, \frac{1}{2}) \quad 0, 0, z$$

$$(2y|0, \frac{1}{2}, \frac{1}{2}) = 2(0, \frac{1}{2}, 0) \quad 0, y, \frac{1}{4}$$

$$(2y|0, \frac{1}{2}, 0) = 2 \qquad x, \frac{1}{4}, 0$$

This layer group, in the coordinate system with basis vectors **b**, **c**, **a** and with an origin shift of **b**/4 has a translational subgroup $\langle 1, 0, 0; 0, 1, 0 \rangle$ and symmetry operations

and the translations and symmetry operations of the layer group become identical with the translations and symmetry operations listed on the page of ITCE (2000) headed by the layer-group-type symbol $p2_12_12$ (L21).

In *ITCE* (2000), there are layer-group types for which there are two or three tabulations, *i.e.* layer groups with two origin choices or three cell choices, respectively. If in *ITCE* (2000) such a layer-group type appears twice, it is listed in Table 2 twice, in both origin choices, or three times, in all three cell choices:

In the final three columns, the rod group isomorphic to $\mathbf{G}/\mathbf{T}_{G2}$ is specified. In the first column, the rod-group type is given. If in the coordinate system of the space group \mathbf{G} the translations and symmetry operations of the rod group are identical with the translations and symmetry operations listed in *ITCE* (2000) on the page headed by the rod-group-type symbol given in the first column, then the basis vectors \mathbf{a} , \mathbf{b} , \mathbf{c} are given in the second column. The third column is then left blank. If not, a change in the basis vectors and/or a shift in origin is required to make the translations and symmetry

operations identical. If required, a new set of basis vectors is given in the second column in terms of the basis vectors of the space group's conventional coordinate system. If required, a shift vector is given in the third column.

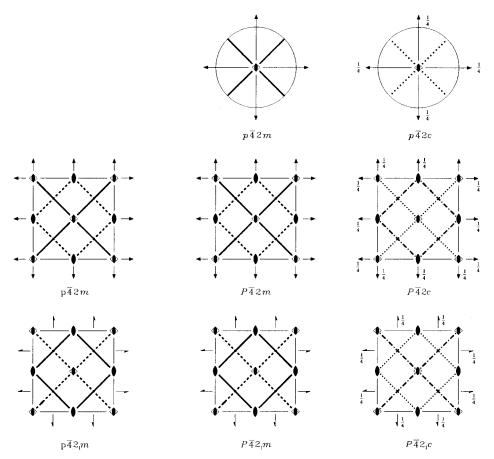
In *ITCE* (2000), there are rod-group types that have tabulated rod groups given in two settings. If such a rod group appears in Table 2, then the acronyms S1 and S2, for *setting 1* and *setting 2*, are used, respectively, to specify the setting.

5. Relationships among diagrams

In Table 2, one finds the following listings of layer groups $\mathbf{G}/\mathbf{T}_{G1}$ and rod groups $\mathbf{G}/\mathbf{T}_{G2}$ isomorphic to factor groups of reducible space groups \mathbf{G} :

G	$\mathbf{G}/\mathbf{T}_{G1}$	$\mathbf{G}/\mathbf{T}_{G2}$
$P\overline{4}2m$	p42 <i>m</i>	$p\bar{4}2m$
$P\bar{4}2c$	$p\bar{4}2m$	$p\bar{4}2c$
$P\bar{4}2_{1}m$	$p\overline{4}2_1m$	$p\overline{4}2m$
$P\bar{4}2_{1}c$	$p\bar{4}2_1m$	$p\overline{4}2c$

One can reformat this information either in the following tabular format



Relationship between symmetry diagrams of reducible space groups and isomorphic layer and rod groups.

research papers

	$p\bar{4}2m$	$p\bar{4}2c$
p42m	$P\overline{4}2m$	$P\bar{4}2c$
$p\bar{4}2_{1}m$	$P\bar{4}2_{1}m$	$P\bar{4}2_{1}c$

or as an array of these groups' corresponding symmetry diagrams, as shown in Fig. 1. In this figure, for each reducible space group \mathbf{G} , the corresponding layer group of the type $\mathbf{G}/\mathbf{T}_{G1}$ is given in the first column of the row containing \mathbf{G} , and the corresponding rod group of the type $\mathbf{G}/\mathbf{T}_{G2}$ in the first row of the column containing \mathbf{G} .

Note in Fig. 1 that the symmetry diagram of the layer group $p\bar{4}2m$ is identical with the symmetry diagram of $P\bar{4}2m$. In general, the symmetry diagram of any layer group is the symmetry diagram of some space group. Consider a layer group \mathbf{L} with its two-dimensional subgroup \mathbf{T}_2 , which, in the conventional coordinate system for layer groups, is in the xy plane. The elements of this layer group can be considered the coset representatives of the factor group $\mathbf{G}/\mathbf{T}_{G1}$ of a space group \mathbf{G} , where \mathbf{T}_{G1} is the one-dimensional translational group $\langle 0,0,1\rangle$. The space group \mathbf{G} has the translational subgroup $\mathbf{T}=\mathbf{T}_{G1}\oplus\mathbf{T}_{G2}$, where $\mathbf{T}_{G2}=\mathbf{T}_2$ and its symmetry operations are identical with the symmetry operations of the layer group \mathbf{L} . The symmetry diagrams of the layer group \mathbf{L} and this space group \mathbf{G} are identical.

The symmetry diagram of the representative rod group of every rod group can be found in the symmetry diagram of some space group. Consider a rod group R with its onedimensional subgroup T_1 , which in the conventional coordinate system for rod groups is in the z direction. The elements of this rod group can be considered the coset representatives of the factor group G/T_{G2} of a space group G, where T_{G2} is the two-dimensional translational group (1, 0, 0; 0, 1, 0). The space group **G** has the translational subgroup $\mathbf{T} = \mathbf{T}_{G1} \oplus \mathbf{T}_{G2}$, where $T_{G1} = T_1$, and its symmetry operations are identical with the symmetry operations of the rod group \mathbf{R} . The symmetry diagram of the rod group **R** is found at the origin of the symmetry diagram of the space group G. For example, in Fig. 1, we see that the symmetry diagram of the rod group of the type $p\bar{4}2m$ (R37) can be found at the origin of the symmetry diagram of the space group of the type $P\bar{4}2m$ (No. 111, D_{2d}^1).

Tables of the layer and rod groups isomorphic to factor groups of reducible space groups can be derived from the space groups' symmetry diagrams using graphical methods analogous to the methods given in §3. For example, for $\mathbf{G} = P\bar{4}2c$ (No. 112, D_{2d}^2) and $\mathbf{T}_{G1} = \mathbf{T}(c)$, one can obtain the symmetry diagram of $\mathbf{G}/\mathbf{T}_{G1}$ [p42m (L57)] from the diagram of the space group. The process of defining elements $G_{i2} = (R_i|T_{i2})$, see §3, in terms of the symmetry diagram of this space group, means (Kopský, 1993):

- (i) replacing each dotted line, representing an axial glide plane with a glide vector normal to the plane of the diagram, with a solid line, representing a mirror plane;
- (ii) replacing each dot-dashed line, representing a diagonal glide plane with a glide vector with one of its components normal to the plane of the diagram, with a dashed line, representing an axial glide plane with a glide vector along the line in the plane of the diagram;
 - (iii) deleting the heights from each of the arrows.

Consequently, one obtains from the symmetry diagram of the space group $P\bar{4}2c$ the symmetry diagram of the layer group $p\bar{4}2m$.

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