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$$x, y, z \quad \bar{x}+1/2, y, z \quad \bar{x}, y+1/2, \bar{z}$$
$$x, y, z \quad \bar{x}, y, z \quad \bar{x}+1/2, y+1/2, \bar{z}.$$

The difference between the two subgroups represented by the one entry is due to the different sets of symmetry operations of **G** which are retained in **S**. This can also be expressed as different conventional origins of **S** with respect to **G**: the two subgroups in the first example above are related by a translation **c**/4 of the origin, and the two subgroups in the second example by **a**/4.

#### *1.2.15.2. Maximal isotypic subgroups and enantiomorphic subgroups of lowest index*

Another set of *klassengleiche* subgroups is that listed under **IIc**, *i.e.* the subgroups **S** which are of the same or of the enantiomorphic subperiodic group type as **G**. Again, one entry may correspond to more than one isotypic subgroup:

(*a*) As in block **IIb**, one entry may correspond to two isotypic subgroups whose difference can be expressed as different conventional origins of **S** with respect to **G**.

(*b*) One entry may correspond to two isotypic subgroups of equal index but with cell enlargements in different directions which are conjugate subgroups in the affine normalizer of **G**. The different vector relationships are given, separated by 'or' and placed within one pair of parentheses; *cf.* example (2).

*Examples*

(1) **G**: Rod group $\not{p}222$ (R13)

**IIc** [2] $\not{p}222$ ($\mathbf{c}' = 2\mathbf{c}$)

This entry corresponds to two isotypic subgroups. Apart from the translations of the enlarged cell, the generators of the subgroups are

$$x, y, z \quad x, \bar{y}, \bar{z} \quad \bar{x}, y, \bar{z}$$
$$x, y, z \quad x, \bar{y}, \bar{z}+1/2 \quad \bar{x}, y, \bar{z}+1/2$$

(2) **G**: Layer group $pmm2$ (L23)

**IIc** [2] $pmm2$ ($\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{b}' = 2\mathbf{b}$)

This entry corresponds to four isotypic subgroups, two with the enlarged cell with $\mathbf{a}' = 2\mathbf{a}$ and two with the enlarged cell with $\mathbf{b}' = 2\mathbf{b}$. The generators of these subgroups are

| | | | | |
|---|---|---|---|---|
| $\mathbf{a}' = 2\mathbf{a}$ | $\mathbf{b}' = \mathbf{b}$ | $x, y, z$ | $\bar{x}, y, z$ | $x, \bar{y}, z$ |
| $\mathbf{a}' = 2\mathbf{a}$ | $\mathbf{b}' = \mathbf{b}$ | $x, y, z$ | $\bar{x}+1/2, y, z$ | $x, \bar{y}, z$ |
| $\mathbf{a}' = \mathbf{a}$ | $\mathbf{b}' = 2\mathbf{b}$ | $x, y, z$ | $\bar{x}, y, z$ | $x, \bar{y}, z$ |
| $\mathbf{a}' = \mathbf{a}$ | $\mathbf{b}' = 2\mathbf{b}$ | $x, y, z$ | $\bar{x}, y+1/2, z$ | $x, \bar{y}, z$ |

(3) **G**: Rod group $\not{p}4_1$ (R24)

**IIc** [3] $\not{p}4_3$ ($\mathbf{c}' = 3\mathbf{c}$)

[5] $\not{p}4_1$ ($\mathbf{c}' = 5\mathbf{c}$)

Listed here are both the maximal isotypic subgroup $\not{p}4_1$ and the maximal enantiomorphic subgroup $\not{p}4_3$, each of lowest index.

#### *1.2.15.3. Minimal non-isotypic non-enantiomorphic supergroups*

If **G** is a maximal subgroup of a group **H**, then **H** is called a minimal supergroup of **G**. Minimal supergroups are again subdivided into two types, the *translationengleiche* or *t* supergroups **I** and the *klassengleiche* or *k* supergroups **II**. For the *t* supergroups **I** of **G**, the listing contains the index [*i*] of **G** in **H** and the *conventional* Hermann–Mauguin symbol of **H**. For the *k* supergroups **II**, the subdivision between **IIa** and **IIb** is not made. The information given is similar to that for the subgroups **IIb**, *i.e.* the relations between the basis vectors of group and supergroup are given, in addition to the Hermann–Mauguin symbols of **H**. Note that either the conventional cell of the *k* supergroup **H** is smaller than that of the subperiodic group **G**, or **H** contains additional centring translations.

*Example: **G**: Layer group $p2_1/m11$ (L15)*

Minimal non-isotypic non-enantiomorphic supergroups:

**I** [2] $pmam$; [2] $pmma$; [2] $pbma$; [2] $pmmn$

**II** [2] $c2/m11$; [2] $p2/m11$ ($2\mathbf{a}' = \mathbf{a}$)

Block **I** lists [2] *pmam*, [2] *pmma* and [2] *pmmn*. Looking up the *subgroup* data of these three groups one finds [2] $p2_1/m11$. Block **I** also lists [2] *pbma*. Looking up the *subgroup* data of this group one finds [2] $p12_1/m1$ ($p2_1/m11$). This shows that the setting of *pbma* does not correspond to that of $p2_1/m11$ but rather to $p12_1/m1$. To obtain the supergroup **H** referred to the basis of $p2_1/m11$, the basis vectors **a** and **b** must be interchanged. This changes *pbma* to *pmba*, which is the correct symbol of the supergroup of $p2_1/m11$.

Block **II** contains two entries: the first where the conventional cells are the same with the supergroup having additional centring translations, and the second where the conventional cell of the supergroup is smaller than that of the original subperiodic group.

#### *1.2.15.4. Minimal isotypic supergroups and enantiomorphic supergroups of lowest index*

No data are listed for *supergroups* **IIc**, because they can be derived directly from the corresponding data of *subgroups* **IIc**.

*Example: **G**: Rod group $\not{p}4_2/m$ (R29)*

The maximal isotypic subgroup of lowest index of $\not{p}4_2/m$ is found in block **IIc**: [3] $\not{p}4_2/m$ ($\mathbf{c}' = 3\mathbf{c}$). By interchanging $\mathbf{c}'$ and **c**, one obtains the minimal isotypic supergroup of lowest index, *i.e.* [3] $\not{p}4_2/m$ ($3\mathbf{c}' = \mathbf{c}$).

### 1.2.16. Nomenclature

There exists a wide variety of nomenclature for layer, rod and frieze groups (Holser, 1961). Layer-group nomenclature includes *zweidimensionale Raumgruppen* (Alexander & Herrmann, 1929*a*,*b*), *Ebenengruppen* (Weber, 1929), *Netzgruppen* (Hermann, 1929*a*), *net groups* (*IT*, 1952; Opechowski, 1986), *reversal space groups in two dimensions* (Cochran, 1952), *plane groups in three dimensions* (Dornberger-Schiff, 1956, 1959; Belov, 1959), *black and white space groups in two dimensions* (Mackay, 1957), (*two-sided*) *plane groups* (Holser, 1958), *Schichtgruppen* (Niggli, 1959; Chapuis, 1966), *diperiodic groups in three dimensions* (Wood, 1964*a*,*b*), *layer space groups* (Shubnikov & Koptsik, 1974), *layer groups* (Köhler, 1977; Koch & Fischer, 1978; Vainshtein, 1981; Goodman, 1984; Litvin, 1989), *two-dimensional* (*subperiodic*) *groups in three-dimensional space* (Brown *et al.*, 1978) and *plane space groups in three dimensions* (Grell *et al.*, 1989).

Rod-group nomenclature includes *Kettengruppen* (Hermann, 1929*a*,*b*), *eindimensionalen Raumgruppen* (Alexander, 1929, 1934), (*crystallographic*) *line groups in three dimensions* (*IT*, 1952; Opechowski, 1986), *rod groups* (Belov, 1956; Vujicic *et al.*, 1977; Köhler, 1977; Koch & Fischer, 1978), *Balkengruppen*

Table 1.2.17.1. *Frieze-group symbols*

| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 |
|---|---|---|---|---|---|---|---|---|---|---|---|
| Oblique | 1 | $p1$ | $r1$ | $r1$ | $r111$ | $(a)$ | $t$ | 1 | $p[1](1)1$ | $r1$ | $p1$ |
| | 2 | $p211$ | $r\bar{1}'$ | $r112$ | $r112$ | $(a):2$ | $t:2$ | 5 | $p[2](1)1$ | $r2$ | $p112$ |
| Rectangular | 3 | $p1m1$ | $r\bar{1}$ | $r1m$ | $rm11$ | $(a):m$ | $t:m$ | 3 | $p[1](1)m$ | $r1m$ | $pm11$ |
| | 4 | $p11m$ | $r11'$ | $rm$ | $r1m1$ | $(a)\cdot m$ | $t\cdot m$ | 2 | $p[1](m)1$ | $r11m$ | $p1m1$ |
| | 5 | $p11g$ | $r_21$ | $rg$ | $r1c1$ | $(a)\cdot\bar{a}$ | $t\cdot a$ | 4 | $p[1](c)1$ | $r11g$ | $p1a1$ |
| | 6 | $p2mm$ | $r\bar{1}1'$ | $rmm2$ | $rmm2$ | $(a):2\cdot m$ | $t:2\cdot m$ | 6 | $p[2](m)m$ | $r2mm$ | $pmm2$ |
| | 7 | $p2mg$ | $r_2\bar{1}$ | $rgm2$ | $rmc2$ | $(a):2\cdot\bar{a}$ | $t:2\cdot a$ | 7 | $p[2](c)m$ | $r2mg$ | $pma2$ |

(Niggli, 1959; Chapuis, 1966), *stem groups* (Galyarskii & Zamorzaev, 1965*a*,*b*), *linear space groups* (Bohm & Dornberger-Schiff, 1966) and *one-dimensional* (*subperiodic*) *groups in three dimensions* (Brown *et al.*, 1978).

Frieze-group nomenclature includes *Bortenornamente* (Speiser, 1927), *Bandgruppen* (Niggli, 1959), *line groups* (*borders*) *in two dimensions* (*IT*, 1952), *line groups in a plane* (Belov, 1956), *eindimensionale 'zweifarbige' Gruppen* (Nowacki, 1960), groups of *one-sided bands* (Shubnikov & Koptsik, 1974), *ribbon groups* (Köhler, 1977), *one-dimensional* (*subperiodic*) *groups in two-dimensional space* (Brown *et al.*, 1978) and *groups of borders* (Vainshtein, 1981).

### 1.2.17. Symbols

The following general criterion was used in selecting the sets of symbols for the subperiodic groups: *consistency with the symbols used for the space groups given in IT* A (2005). Specific criteria following from this general criterion are as follows:

(1) The symbols of subperiodic groups are to be of the Hermann–Mauguin (international) type. This is the type of symbol used for space groups in *IT* A (2005).

(2) A symbol of a subperiodic group is to consist of a letter indicating the lattice centring type followed by a set of characters indicating symmetry elements. This is the format of the Hermann–Mauguin (international) space-group symbols in *IT* A (2005).

(3) The sets of symmetry directions and their sequences in the symbols of the subperiodic groups are those of the corresponding space groups. Layer and rod groups are three-dimensional subperiodic groups of the three-dimensional space groups, and frieze groups are two-dimensional subperiodic groups of the two-dimensional space groups. Consequently, the symmetry directions and sequence of the characters indicating symmetry elements in layer and rod groups are those of the three-dimensional space groups; in frieze groups, they are those of the two-dimensional space groups, see Table 1.2.4.1 above and Table 2.2.4.1 of *IT* A (2005). Layer groups appear as subgroups of three-dimensional space groups, as factor groups of three-dimensional reducible space groups (Kopský, 1986, 1988, 1989*a*,*b*, 1993; Fuksa & Kopský, 1993) and as the symmetries of planes which transect a crystal of a given three-dimensional space-group symmetry. For example, the layer group *pmm*2 is a subgroup of the three-dimensional space group *Pmm*2; is isomorphic to the factor group $Pmm2/\mathrm{T}_z$ of the three-dimensional space group *Pmm*2, where $\mathrm{T}_z$ is the translational subgroup of all translations along the *z* axis; and is the symmetry of the plane transecting a crystal of three-dimensional space-group symmetry *Pmm*2, perpendicular to the *z* axis, at $z = 0$. In these examples, the symbols for the three-dimensional space group and the related subperiodic layer group differ only in the letter indicating the lattice type.

A survey of sets of symbols that have been used for the subperiodic groups is given below. Considering these sets of symbols in relation to the above criteria leads to the sets of symbols for subperiodic groups used in Parts 2, 3 and 4.

#### *1.2.17.1. Frieze groups*

A list of sets of symbols for the frieze groups is given in Table 1.2.17.1. The information provided in this table is as follows:

Columns 1 and 2: sequential numbering and symbols used in Part 2.

Columns 3, 4 and 5: symbols listed by Opechowski (1986).

Column 6: symbols listed by Shubnikov & Koptsik (1974).

Column 7: symbols listed by Vainshtein (1981).

Columns 8 and 9: sequential numbering and symbols listed by Bohm & Dornberger-Schiff (1967).

Column 10: symbols listed by Lockwood & Macmillan (1978).

Column 11: symbols listed by Shubnikov & Koptsik (1974).

Sets of symbols which are of a non-Hermann–Mauguin (international) type are the set of symbols of the 'black and white' symmetry type (column 3) and the sets of symbols in columns 6 and 7. The sets of symbols in columns 4, 5 and 11 do not follow the sequence of symmetry directions used for two-dimensional space groups. The sets of symbols in columns 3, 4, 5 and 10 do not use a lower-case script *p* to denote a one-dimensional lattice. The set of symbols in column 9 uses parentheses and square brackets to denote specific symmetry directions. The symbol *g* is used in Part 1 to denote a glide line, a standard symbol for two-dimensional space groups (*IT* A, 2005). A letter identical with a basis-vector symbol, *e.g.* *a* or *c*, is not used to denote a glide line, as is done in the symbols of columns 5, 6, 7, 9 and 11, as such a letter is a standard notation for a three-dimensional glide plane (*IT* A, 2005).

Columns 2 and 3 show the isomorphism between frieze groups and one-dimensional magnetic space groups. The one-dimensional space groups are denoted by $p1$ and $p\bar{1}$. The list of symbols in column 3, on replacing *r* with *p*, is the list of one-dimensional magnetic space groups. The isomorphism between these two sets of groups interexchanges the elements $\bar{1}$ and $1'$ of the one-dimensional magnetic space groups and, respectively, the elements $m_x$ and $m_y$, mirror lines perpendicular to the [10] and [01] directions, of the frieze groups.

#### *1.2.17.2. Rod groups*

A list of sets of symbols for the rod groups is given in Table 1.2.17.2. The information provided in the columns of this table is as follows:

Columns 1 and 2: sequential numbering and symbols used in Part 3.

Columns 3 and 4: sequential numbering and symbols listed by Bohm & Dornberger-Schiff (1966, 1967).

Columns 5, 6 and 7: sequential numbering and two sets of symbols listed by Shubnikov & Koptsik (1974).



references