International Tables for Crystallography (2006). Vol. E, Section 5.2.3.1.4, pp. 400–401.

by horizontal lines through the last three columns. Two ways are used to express the fact that the origin of the scanning group does not coincide with the origin of the original group $\mathcal{G}$. We use the Hermann–Mauguin symbol of the scanning group with the statement of the shift of its origin (as a rule below the symbol) for each of the separated blocks. In some cases, for typographical reasons, we state with respect to which origin the Hermann–Mauguin symbol of the scanning group, and consequently the description of the translation orbit and of the sectional layer groups, is referring to.

5.2.3.1.4. *The linear orbits and sectional layer groups*

The fourth column, headed *Linear orbit* $s\mathbf{d}$, describes the linear orbits of planes for the orientation of this row and the fifth column, headed *Sectional layer group* $\mathcal{L}(s\mathbf{d})$, describes the corresponding sectional layer groups.

The location of the plane along the line $P + s\mathbf{d}$ determines a certain layer group; the symbol $\mathcal{L}(s\mathbf{d})$ next to $s\mathbf{d}$ is a shorthand for the sectional layer group $\mathcal{L}(P + s\mathbf{d}, (hkl))$ of the section plane passing through the point $P + s\mathbf{d}$ on the scanning line. $\mathcal{L}(s\mathbf{d})$, as a function of s, has a periodicity of the translation normalizer of the space group $\mathcal{G}$ in the direction $\mathbf{d}$ but we list the translation orbits within $0 \le s < 1$, *i.e.* with periodicity $\mathbf{d}$. This is important because the planes at levels separated by the periodicity of the normalizer do not necessarily belong to the same orbit.

The planes form orbits with fixed parameter s and with a variable parameter s. The orbits with fixed parameter s are recorded in terms of fractions of vector $\mathbf{d}$; one of these fractions always lies in the interval $0 \le s < s_o$, where s_o is the length of the fundamental region of the scanned group $\mathcal{G}$ along the scanning line $P + s\mathbf{d}$ in units of $\mathbf{d}$. The fixed values of s are always given in the range $0 \le s < 1$. If planes at different levels belong to the same orbit, then the levels are enclosed in square brackets. The sectional layer group corresponding to a certain level s is then given in the fifth column by its Hermann–Mauguin symbol in the coordinate system $(P + s\mathbf{d}; \mathbf{a}', \mathbf{b}', \mathbf{d})$. If the levels on the same line refer to the same Hermann–Mauguin symbol of a sectional layer group but are not enclosed in brackets, then they belong to different orbits. The sectional layer groups belonging to different planes of the orbit are certainly of the same type and parameters but they may be oriented or located in different ways so that their Hermann–Mauguin symbols are different because they refer to the same basis $(\mathbf{a}', \mathbf{b}')$. In this case, the levels corresponding to the same orbit are listed in a column, beginning and ending with brackets, and to each level is given the sectional layer group.

There is always only one row (which may, however, split for typographical reasons) corresponding to orbits with a variable parameter s and the one sectional layer group which is floating along the scanning direction and which is a common subgroup of all sectional layer groups for orbits with fixed parameters. This row always contains the term $s\mathbf{d}$ where s belongs to the fundamental region $0 \le s < s_o = \frac{1}{f}$ of the group $\mathcal{G}$ along the line $P + s\mathbf{d}$. Here s_o is a fraction of 1 and the region is a fraction of the interval $0 \le s < 1$. These levels correspond to locations of planes of the translation orbit along the direction $\mathbf{d}$ within the unit interval. The levels are expressed in a compact way; as a result there appears an entry $\pm s\mathbf{d}$ in cases when the scanning group is not polar. Since s is in the interval $0 \le s < s_o$, $-s$ is negative and hence not in the interval $0 \le s_i < 1$; this level is equivalent to the level $(1 - s)\mathbf{d}$.

Following each Hermann–Mauguin symbol, we give the sequential number of the type to which the sectional layer group belongs, according to its numbering in Parts 1–4 of this volume.

Example 1: Orientation orbit (001) for the space groups $P422$, D_4^1 (No. 89), $P4_222$, D_4^5 (No. 93) and $P4_122$, D_4^3 (No. 91).

Group $P422$: The entries '$0\mathbf{d}, \frac{1}{2}\mathbf{d}$' in the fourth column followed by $p422$ in the fifth column indicate that there are two separate translation orbits, represented by planes passing through P and $P + \frac{1}{2}\mathbf{d}$; planes of both orbits have the same sectional layer group with reference to the respective coordinate systems.

The sectional layer symmetry at a general level is $p4$ and the translation orbit contains planes at two levels (the index of the point group 4 in the point group 422), described as $[s\mathbf{d}, -s\mathbf{d}]$. It is $s_o = \frac{1}{2}$ and both levels $\pm s\mathbf{d}$ belong to the same orbit. For positive s we can change $-s$ to $(1 - s)$ to get the level in the interval $0 \le s_i < 1$.

Group $P4_222$: The entries $[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$ are now enclosed between square brackets to indicate that the planes at these levels along the line $P + s\mathbf{d}$ belong to the same orbit. The sectional layer symmetry is $p222$.

The sectional layer symmetry at a general level is $p112$, so that there must be four $[422\ (D_4) : 122\ (C_2)]$ levels which are described as $[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$ where $0 < s < s_o = \frac{1}{4}$. Again we can change $-s$ to $(1 - s)$ to get the level in the interval $0 < s_i < 1$.

Group $P4_122$: The entry '$[0\mathbf{d}, \frac{1}{2}\mathbf{d}$;' in the first subrow and the entry '$\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$' in the second subrow indicate that the planes on corresponding levels all belong to the same translation orbit. The corresponding sectional layer groups $p121$ and $p211$ for the first and second subrow are of the same type but the orientations of their twofold axes are different. The Hermann–Mauguin symbols are therefore different because they are expressed with reference to the same basis [in this case the basis $(\mathbf{a}, \mathbf{b})$].

The sectional layer symmetry at a general level is $p1$ so that $s_o = \frac{1}{8}$ and there must be eight levels which are described as $[\pm s\mathbf{d}, (\pm s + \frac{1}{4})\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}, (\pm s + \frac{3}{4})\mathbf{d}]$.

Example 2: We consider the group $R\bar{3}$, C_{3i}^2 (No. 148) and the orientation (0001). There are three subrows in the columns for the translation orbits and the sectional layer groups. In the first row there are the entries $[0\mathbf{d}$, $[\frac{1}{2}\mathbf{d}$; and $p\bar{3}$; in the second row $\frac{1}{3}\mathbf{d}$, || $\frac{5}{6}\mathbf{d}$, and $p\bar{3}$ $[(2\mathbf{a} + \mathbf{b})/3]$; and in the third row $\frac{2}{3}\mathbf{d}]$ $\frac{1}{6}\mathbf{d}]$ and $p\bar{3}$ $[(\mathbf{a} + 2\mathbf{b})/3]$. This is to be interpreted as follows: the levels $[0\mathbf{d}, \frac{1}{3}\mathbf{d}$ and $\frac{2}{3}\mathbf{d}]$ belong to one translation orbit, distinct from the orbit to which belong the levels $[\frac{1}{2}\mathbf{d}, \frac{5}{6}\mathbf{d}$ and $\frac{1}{6}\mathbf{d}]$. The sectional layer groups are groups $p\bar{3}$ on all these levels but they are located at different distances from points $P + s\mathbf{d}$ for different levels $s\mathbf{d}$.

The sectional layer symmetry at a general level is $p3$. The point group 3 is of index 2 in the point group $\bar{3}$ and the lattice is of the type R so there are six planes in the translation orbit per unit interval along $\mathbf{d}$ and $s_o = \frac{1}{6}$. The translation orbit is described by $[\pm s\mathbf{d}, (\pm s + \frac{1}{3})\mathbf{d}, (\pm s + \frac{2}{3})\mathbf{d}]$.

Example 3: Space group $P4/mmm$, D_{4h}^1 (No. 123). The scanning groups for the orientations (100) and (010) which belong to the same orientation orbit are expressed by the same Hermann–Mauguin symbol $Pmmm$ in their respective bases. The translation orbits and sectional layer groups are therefore expressed in the same block.

The scanning groups for the orientations (110) and $(1\bar{1}0)$ of the same orientation orbit under the space group $P4/nbm$, D_{4h}^3 (No. 125) are expressed by the same Hermann–Mauguin symbol $Bmcm$ ($\mathbf{d}$/4) in the respective bases if the scanned group is chosen according to origin choice 1 in *IT* A. Hence the translation orbits and sectional layer groups are expressed in one block; they are the same with reference to their corresponding bases. For origin choice 2, the locations of the scanning groups are different; we obtain the group $Bmcm$ for the orientation (110) and $Bmcm$ $[(\mathbf{a}' + \mathbf{d})/4]$ for the orientation $(1\bar{1}0)$. Each of these scanning groups has its own box with the translation orbits and sectional layer groups. If we compare the two boxes, we observe that the data in the second box are the same as in the first box but shifted by $[(\mathbf{a}' + \mathbf{d})/4]$.

Example 4: Consider the block of the orientation orbit (111), $(\bar{1}11)$, $(1\bar{1}1)$, $(11\bar{1})$ for space groups $P4_332$, O^6 (No. 212), $P4_132$, O^7 (No. 213) and $I4_132$, O^8 (No. 214). The Hermann–Mauguin symbol of the scanning group with reference to their bases is the same, $R32$, up to a shift of the origin. In the row for each orientation, therefore not only are the bases given, but also the location of the origin so that a complete coordinate system is specified in such a way that the symbol is exactly the same for each orientation. The symbol of the scanning group, the location of the orbits and the sectional layer groups are given in the last block; all this information is formally the same but for each orientation it refers to its own coordinate system.

5.2.3.2. *Auxiliary tables*

The auxiliary tables describe cases of monoclinic/inclined scanning for groups of orthorhombic and higher symmetries. They are clustered together for groups of each Laue class, starting from Laue class D_{2h} – mmm, after the tables of orthogonal scanning, *i.e.* after the standard-format tables for this Laue class.

All possible cases of monoclinic/inclined scanning reduce to cases where the scanned group $\mathcal{G}$ itself is monoclinic and the orientation is defined by the Miller indices $(mn0)$. These cases are described as a part of the standard-format tables for monoclinic groups. Two bases are used in this description:

(i) The conventional basis $(\mathbf{a}, \mathbf{b}, \mathbf{c})$ of the group $\mathcal{G}$ in its role as the scanned group.

(ii) The conventional basis (in the sense of the convention for scanning groups, see Section 5.2.2.3) $(\mathbf{a}', \mathbf{b}', \mathbf{d})$ of the group $\mathcal{H} = \mathcal{G}$ in its role as the scanning group.

If the scanned group $\mathcal{G}$ is of higher than monoclinic symmetry, then the monoclinic scanning group $\mathcal{H} \subset \mathcal{G}$ and we use three bases:

(i) The conventional basis $(\mathbf{a}, \mathbf{b}, \mathbf{c})$ of the scanned group $\mathcal{G}$.

(ii) The conventional basis $(\widehat{\mathbf{a}}, \widehat{\mathbf{b}}, \widehat{\mathbf{c}})$ of the monoclinic scanning group $\mathcal{H}$, which is further called the *auxiliary basis*. This basis is always chosen so that the vector $\widehat{\mathbf{c}}$ is the unique axis vector.

(iii) The conventional basis (in the sense of the convention for scanning groups, see Section 5.2.2.3) $(\mathbf{a}', \mathbf{b}', \mathbf{d})$ of the scanning group $\mathcal{H}$.

Two types of tables from which orbits of planes and sectional layer groups can be deduced are given:

(1) *Tables of orientation orbits and auxiliary bases of scanning groups*. These contain Miller indices of orientations in the orbit and define auxiliary bases $(\widehat{\mathbf{a}}, \widehat{\mathbf{b}}, \widehat{\mathbf{c}})$ of the respective scanning groups in terms of the basis $(\mathbf{a}, \mathbf{b}, \mathbf{c})$ of the scanned group $\mathcal{G}$ and of the Miller indices of the orientation.

(2) *Reference tables*. These serve to give a reference to that table of a monoclinic group from which one can read the scanning data.

In the next two sections we describe the construction of these two types of tables and their use in detail.

5.2.3.2.1. *Tables of orientation orbits and auxiliary bases of scanning groups*

The cases of monoclinic/inclined scanning occur when the orientation of the section plane:

(i) contains the direction of some symmetry axis of even order [scanning group of geometric class 2 (C_2)],

(ii) is orthogonal to a symmetry plane [scanning group of geometric class m (C_s)],

(iii) contains the direction of some symmetry axis of even order and at the same time is orthogonal to a symmetry plane [scanning group of geometric class $2/m$ (C_{2h})].

Auxiliary basis of the scanning group. In each of these cases, there is a set of orientations for which the property (i), (ii) or (iii) is common and all orientations of this set contain the vector that defines the unique axis of a monoclinic scanning group which is also common for all orientations of the set. An auxiliary basis $(\widehat{\mathbf{a}}, \widehat{\mathbf{b}}, \widehat{\mathbf{c}})$ of this scanning group is defined with reference to that one orientation of the set which is described by Miller indices $(mn0)$.

The first column of each table describes orientations of the orbit by Miller indices with reference to the conventional basis $(\mathbf{a}, \mathbf{b}, \mathbf{c})$ of the scanned group $\mathcal{G}$. Various possible situations can be distinguished by three criteria:

(1) The structure of orbits.

(i) All orientations of the orbit contain the vector of the unique axis of the scanning group. This also means that there is only one scanning group for all orientations of the orbit.

This situation occurs for orientations that contain the vector of principal axis c in tetragonal and hexagonal groups. It occurs also for orientations which contain the vector of any of the orthorhombic axes c, a or b.

(ii) The orbit splits into sets of orientations where each set has its own common unique axis and scanning group.

This situation occurs for orientations that contain vectors of auxiliary axes of groups of Laue classes $4/mmm$ (D_{4h}), $\bar{3}m$ (D_{3d}), $6/mmm$ (D_{6h}), $m\bar{3}$ (T_h) and $m\bar{3}m$ (O_h).

(2) Possible increase of the symmetry for special orientations.

(i) All orientations of the set with common unique axis have the same monoclinic scanning group.

This is the case of groups of Laue classes $4/m$ (C_{4h}) and $6/m$ (C_{6h}), and of orientations that contain the vector $\mathbf{c}$ of the principal axis.

(ii) In all other cases there appear special orientations in the set which have higher symmetry than monoclinic.

(3) Auxiliary basis of the scanning group.

The auxiliary bases of scanning groups are their conventional bases corresponding to unique axis c.

(i) If the conventional basis of the scanning group can be based on the same vectors as the conventional basis of the scanned group, parameters m, n are used in the Miller indices that define the orientation.

(ii) If the conventional basis of the scanning group cannot be based on the same vectors as the conventional basis of the scanned group, parameters h, k, l are used in the Miller indices that define the orientation with reference to the conventional basis $(\mathbf{a}, \mathbf{b}, \mathbf{c})$.

In these cases, the transformation of Miller indices with reference to the conventional basis $(\mathbf{a}, \mathbf{b}, \mathbf{c})$ to Miller indices with reference to auxiliary basis $(\widehat{\mathbf{a}}, \widehat{\mathbf{b}}, \widehat{\mathbf{c}})$ is given in a row under the orientation orbit. The letters m and n are always used for Miller indices with reference to auxiliary bases.

The second column assigns to each orientation the conventional basis $(\mathbf{a}', \mathbf{b}', \mathbf{d})$ of the monoclinic scanning group that is related to the auxiliary basis $(\widehat{\mathbf{a}}, \widehat{\mathbf{b}}, \widehat{\mathbf{c}})$ given in the third column in the same way as to the standard basis $(\mathbf{a}, \mathbf{b}, \mathbf{c})$ in the case of monoclinic groups.

The conventional basis $(\mathbf{a}', \mathbf{b}', \mathbf{d})$ is always chosen so that its first vector $\mathbf{a}'$ is the vector of the common unique axis. Vector $\mathbf{b}'$ is defined by the orientation of section planes and hence by Miller indices (either directly or indirectly through transformation to a monoclinic basis). There is the same freedom in the choice of the scanning direction $\mathbf{d}$ as in the cases of monoclinic/inclined scanning in the case of monoclinic groups.

5.2.3.2.2. *Reference tables*

Each table of orientation orbits for a certain centring type(s) is followed by reference tables which are organized by arithmetic classes belonging to this centring type(s). The scanned space groups $\mathcal{G}$ are given in the first row by their sequential number, Schönflies symbol and short Hermann–Mauguin symbol. They are arranged in order of their sequential numbers unless there is a clash with arithmetic classes; a preference is given to collect groups of the same arithmetic class in one table. If space allows it, groups of more than one arithmetic class are described in one table.

references