International Tables for Crystallography (2010). Vol. E, Section 5.2.3, pp. 401–405.

The difference between monoclinic/orthogonal and monoclinic/inclined scanning is illustrated in Fig. 5.2.2.2. The orientation in the first case is fixed, while the second case applies to various orientations containing the monoclinic unique axis. The orientation can be defined by one free parameter, the angle φ; we use instead Miller indices ($mn0$).

5.2.3. The contents and arrangement of the scanning tables

In the scanning tables two formats are used:

Standard format: This is the format in which the complete tables for triclinic and monoclinic groups and the tables of orthogonal scanning for all other groups are presented.

Auxiliary tables: These tables represent, in an abbreviated form, the cases where the scanned group is orthorhombic or belongs to a higher system and the orientation defines monoclinic/inclined scanning. The scanning is represented implicitly by referring to respective tables of monoclinic groups. [Note that in the online version of this volume the auxiliary tables are supplemented by explicit scanning tables.]

The tables are grouped according to crystallographic systems. Within each system, the standard-format tables are grouped into geometric classes in the same order as in *IT* A. The auxiliary tables follow the tables of standard format at the end of each Laue class.

5.2.3.1. *The standard format*

The content and arrangement of the standard-format tables are as follows:

(1) Headline.
(2) Orientation orbit.
(3) Conventional basis of the scanning group.
(4) Scanning group.
(5) Translation orbit.
(6) Sectional layer group.

The standard tables for triclinic groups describe the trivial scanning where the scanning group is $P1$ or $P\bar{1}$. The tables for monoclinic groups describe monoclinic/orthogonal scanning and monoclinic/inclined scanning. The standard tables for the remaining groups describe only orthogonal scanning for these groups.

5.2.3.1.1. *Headline*

The headline begins with the serial number of the space-group type identical with the numbering given in *IT* A, followed by a short Hermann–Mauguin symbol. The Schönflies symbol is given in the upper right-hand corner.

The next line is centred and contains the full Hermann–Mauguin symbol of the specific space group for which the scanning is described in the table. This is followed by a statement of origin in those cases where two space groups of different origin are considered, or by a statement of cell choice when different cell choices are used for a monoclinic space group.

The specific space group considered in the table is that space group, including its orientation (setting) and location (origin choice), the diagram of which is presented in *IT* A, assuming that the upper left-hand corner of the diagram represents the origin P, its left edge downwards the vector $\mathbf{a}$, its upper edge to the right the vector $\mathbf{b}$, while vector $\mathbf{c}$ is directed upwards. In the case of orthorhombic and monoclinic groups, this is the diagram in the (abc) setting, the so-called standard setting. For some group types, two different origins are given in *IT* A. Both are used to consider two specific groups of the same type with different locations in the present tables. The scanning for each of these groups is described in a separate table. In the case of monoclinic groups, one, three or six different cell choices, depending on the group type, are considered, see Section 5.2.4.2.

5.2.3.1.2. *Orientation orbit*

Each table is divided into five columns. The first column is entitled *Orientation orbit* (hkl) or *Orientation orbit* ($hkil$). The orientations are specified by their Miller or Bravais–Miller indices. Each orientation defines a row for which the scanning is described in the next columns. Orientations which belong to the same orbit are grouped together and orientation orbits are separated by horizontal double lines across the table for space groups of the tetragonal and higher-symmetry systems and for the monoclinic groups. The vertical separation for orthorhombic groups is explained in Section 5.2.4.3.

Orientation orbits are listed in each table in the following order from top to bottom:

(1) Special orientation orbits with fixed parameters which contain just one orientation. Such orbits do not occur in triclinic and cubic groups.

(2) Special orientation orbits with fixed parameters which contain several orientations. Such orbits do not occur in triclinic, monoclinic and orthorhombic groups.

(3) Special orientation orbits with variable parameter. Such orbits do not occur in triclinic groups. They are presented in standard format for monoclinic groups. In this case, the orientations are defined by Miller indices ($n0m$) (unique axis b) or ($mn0$) (unique axis c) and the orbit contains just one orientation. For higher symmetries, these orbits contain several orientations which are given in the auxiliary tables.

General orientation orbits are not included; the corresponding scanning is trivial and the presentation of these orbits would take up too much space.

5.2.3.1.3. *The scanning group and its conventional basis*

The second column is entitled *Conventional basis of the scanning group* and it contains three subcolumns headed by the symbols of vectors $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{d}$. Next to it is the third column with the heading *Scanning group* $\mathcal{H}$. In the subcolumns, the vectors $\mathbf{a}'$, $\mathbf{b}'$ and $\mathbf{d}$ of the conventional bases of the scanning groups $\mathcal{H}$ are specified in terms of the conventional basis ($\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$) of the scanned group $\mathcal{G}$. The scanning groups are described in the third column by their short Hermann–Mauguin symbols.

(1) *Orbits with one orientation*: With the exception of cubic groups, all space groups are reducible so that the orientations (001) or (0001) are invariant under the point group G and the orbit contains only one orientation. The scanning group $\mathcal{H}$ in these cases is identical with the scanned group $\mathcal{G}$ and its conventional basis ($\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{d}$) is identical with the conventional basis ($\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$) so that the groups $\mathcal{G}$ and $\mathcal{H}$ are denoted by the same Hermann–Mauguin symbol. The row for this orientation is always listed first.

The scanning group $\mathcal{H}$ also coincides with the scanned group $\mathcal{G}$ for the orientations (100) and (010) in orthorhombic groups. However, the Hermann–Mauguin symbol for the scanning group may differ from that of the scanned group. This is a result of having the $\mathbf{a}'$ and $\mathbf{b}'$ basis vectors of the scanning group always representing the basis vectors of the resulting sectional layer groups. The alternative setting symbols used are those listed in Table 4.3.2.1 of Part 4 of *IT* A.

Example

Space group *Pbcn*, D_{2h}^{14} (No. 60). The group itself is the scanning group for all three orientations (001), (100) and (010). However, in view of the conventional choice of the basis of the scanning group, its symbols are *Pbcn*, *Pbna* and *Pnca*, respectively.

Monoclinic groups. The scanning group $\mathcal{H}$ coincides with the scanned group $\mathcal{G}$ for the orientations (010) (unique axis *b*) and (001) (unique axis *c*). These are the cases of monoclinic/orthogonal scanning and, according to convention, the scanning vector **d** is chosen as the vector of the unique axis. The symbol of the scanning group coincides with the Hermann–Mauguin symbol for unique axis *c* in both cases.

The scanning group $\mathcal{H}$ also coincides with the scanned group $\mathcal{G}$ for orientations (*n*0*m*) (unique axis *b*) or (*mn*0) (unique axis *c*). These cases lead to monoclinic/inclined scanning described below in conjunction with the auxiliary tables. Vector $\mathbf{a}'$ is, in these cases, chosen as the vector of the unique axis. Since this vector is considered as the first vector in the conventional basis of the scanning group, the Hermann–Mauguin symbols for the scanning group are the symbols that correspond to unique axis *a*. They may differ further depending on the choice of vectors $\mathbf{b}'$ and **d**.

(2) *Orbits with several orientations*: There are several Miller indices in each box of the first column which denote the orientations belonging to one orientation orbit. In the three subcolumns of the second column, the conventional bases of the scanning groups $\mathcal{H}_i$, *i.e.* the vectors $\mathbf{a}'_i$, $\mathbf{b}'_i$, $\mathbf{d}_i$, are specified in terms of the conventional basis vectors **a**, **b**, **c** of the space group $\mathcal{G}$ and of the Miller indices. The vectors $\mathbf{a}'_i$, $\mathbf{b}'_i$, $\mathbf{d}_i$ then represent the conventional bases with respect to which the scanning groups $\mathcal{H}_i$ are given by their Hermann–Mauguin symbols in the third column. These scanning groups are of the same type for all orientations of the orbit and they are also oriented in the same way with respect to their bases; they may, however, have different origins. Therefore, the Hermann–Mauguin symbols of the scanning groups are the same for all orientations of a given orbit up to a possible shift of origin.

Example

Space groups $P42_12$, D_4^2 (No. 90), $P4_122$, D_4^3 (No. 91) and $P4_12_12$, D_4^4 (No. 92), the orientation orbit (100) and (010): In the case of the group $P42_12$, the scanning groups for the orientations (100) and (010) are denoted by the same symbol $P2_122_1$ with reference to coordinate systems $(P; \mathbf{a}', \mathbf{b}', \mathbf{d}) = (P; \mathbf{b}, \mathbf{c}, \mathbf{a})$ and $(P; \mathbf{a}', \mathbf{b}', \mathbf{d}) = (P; -\mathbf{a}, \mathbf{c}, \mathbf{b})$, respectively.

In the case of the group $P4_122$, the scanning group for the orientation (100) is written as $P22_12$ $(\mathbf{b}'/4)$. This is equivalent to the statement that the scanning group is the group $P22_12$ with reference to coordinate system $(P + \mathbf{b}'/4; \mathbf{a}', \mathbf{b}', \mathbf{d}) = (P + \mathbf{c}/4; \mathbf{b}, \mathbf{c}, \mathbf{a})$. The scanning group for the orientation (010) is the group $P22_12$ with reference to coordinate system $(P; \mathbf{a}', \mathbf{b}', \mathbf{d}) = (P; -\mathbf{a}, \mathbf{c}, \mathbf{b})$.

In the case of the group $P4_12_12$, we conclude analogously that the scanning group for the orientation (100) is the group $P2_12_12_1$ with reference to coordinate system $(P + 3\mathbf{b}'/8 + \mathbf{d}/4; \mathbf{a}', \mathbf{b}', \mathbf{d}) = (P + 3\mathbf{c}/8 + \mathbf{a}/4; \mathbf{b}, \mathbf{c}, \mathbf{a})$, while for the orientation (010) it is the group $P2_12_12_1$ with reference to coordinate system $(P + \mathbf{b}'/8 + \mathbf{d}/4; \mathbf{a}', \mathbf{b}', \mathbf{d}) = (P + \mathbf{c}/8 + \mathbf{b}/4; -\mathbf{a}, \mathbf{c}, \mathbf{b})$.

The vectors $\mathbf{a}'_i$, $\mathbf{b}'_i$ also define the translation subgroup T_{Gi} of all sectional layer groups corresponding to a given orientation, which are listed in the fifth column. The vectors either themselves constitute the conventional basis of these layer groups or the conventional basis is expressed through them.

The scanning groups $\mathcal{H}_i$ are conjugate subgroups of the space group $\mathcal{G}$ in cases when there is more than one orientation in the orbit. They are accordingly expressed by the same Hermann–Mauguin symbol with respect to different coordinate systems. There are cases when the origins of these coordinate systems for the conjugate scanning groups $\mathcal{H}_i$ coincide. In this case, one block of the table is sufficient to describe the scanning groups, the translation orbits and the corresponding sectional layer groups in the same manner as in the case of an orbit with one orientation. The common origin $P + \boldsymbol{\tau}$ is stated in a line above the block in the form 'With respect to origin at $P + \boldsymbol{\tau}$' if it is different from the origin *P* of the coordinate system of the scanned group $\mathcal{G}$.

When origins are different, there appear several blocks with Hermann–Mauguin symbols of the scanning group at different locations for different orientations. The blocks are then separated 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***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 **d** but we list the translation orbits within $0 \le s < 1$, *i.e.* with periodicity **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 **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 **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 $0 \leq s < s_o = \frac{1}{f}$ 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 $0 \leq s < 1$. These levels correspond to locations of planes of the translation orbit along the direction **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 $0 \leq s < s_o$, $-s$ is negative and hence not in the interval $0 \leq s_i < 1$; 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 $0 \leq s_i < 1$.

Group P4₂22: 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 P4₁22: 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**a** + **b**)/3]; and in the third row $\frac{2}{3}\mathbf{d}] \frac{1}{6}\mathbf{d}]$ and $p\bar{3}$ [(**a** + 2**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 **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 $Bmcm$ (**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.

The first column is identical with the first column of the table of orientation orbits. On the intersection of a column which specifies the scanned group $\mathcal{G}$ and of a row which specifies the orientation by its Miller (Bravais–Miller) indices is found the scanning group, given by its Hermann–Mauguin symbol with reference to the auxiliary basis $(\widehat{\mathbf{a}}, \widehat{\mathbf{b}}, \widehat{\mathbf{c}})$. This symbol, which may also contain a shift of origin, instructs us which monoclinic scanning table to consult. The vectors $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{d}$ that determine the lattice of sectional layer groups and the scanning direction are those given in the table of orientation orbits. Depending on the values of parameters m, n, p, q we find the scanning group in its basis ($\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{d}$) and the respective sectional layer groups.

5.2.4. Guidelines for individual systems

5.2.4.1. Triclinic system

The triclinic groups are trivial even from the viewpoint of scanning but it is nontrivial to express the vectors $\mathbf{a}'$, $\mathbf{b}'$ and $\mathbf{d}$ in terms of vectors $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ and of Miller indices (hkl). Since the groups are related in the same way with respect to any given basis, we do not identify bases in the two tables. The specification *Any admissible choice* for the scanning group means that the vectors $\mathbf{a}'$, $\mathbf{b}'$ have to be chosen as a basis of the translation group in the subspace defined by Miller indices and $\mathbf{d}$ should be the vector that completes the basis of the translation group in the whole space.

The scanned groups are identical with the scanning group for all orientations in the triclinic groups $P1$, C_1^1 (No. 1) and $P\bar{1}$, C_i^1 (No. 2). There is only one orientation in each orientation orbit. In the case of the group $P1$, C_1^1 (No. 1), there is one type of linear orbit consisting of planes generated by translations $\mathbf{d}$ from either one of the set and the respective layer symmetries are the trivial groups $p1$ (L01). In the case of the group $P\bar{1}$, C_i^1 (No. 2), the orbit with a general location consists of a pair of planes, located symmetrically from a symmetry centre at distances $\pm s$ in the scanning direction $\mathbf{d}$, which is then periodically repeated with periodicity $\mathbf{d}$; the sectional layer symmetry of these planes is $p1$ (L01). Furthermore, there are two linear orbits corresponding to positions $0\mathbf{d}$ and $\frac{1}{2}\mathbf{d}$, each of which consists of a periodic set of planes with periodicity $\mathbf{d}$; the sectional symmetry in each of these cases is $p\bar{1}$ (L02).

The triclinic scanning also applies to general orientation orbits of all space groups of higher symmetry than triclinic. If the space group $\mathcal{G}$ is noncentrosymmetric, then the number of orientations in the orientation orbit is the order $|G|$ of the point group G and the linear orbits are described for each orientation as in the case of the group $P1$, C_1^1 (No. 1). If the space group $\mathcal{G}$ is centrosymmetric, then the number of orientations in the orientation orbit is $|G|/2$ and the linear orbits are described for each orientation as in the case of the group $P\bar{1}$, C_i^1 (No. 2).

5.2.4.2. Monoclinic system

The scanning of monoclinic groups is nontrivial if the section planes are either orthogonal to or parallel with the unique axis. The first case results in monoclinic/orthogonal scanning, the second in monoclinic/inclined scanning.

Depending on the space-group type, a monoclinic group $\mathcal{G}$ admits one, three or six cell choices, which are illustrated and labelled by numbers 1, 2, 3 and $\tilde{1}$, $\tilde{2}$, $\tilde{3}$ in Fig. 5.2.4.1. For each cell choice, a separate table is given in which the group is specified by Hermann–Mauguin symbols with reference to unique axis b or to unique axis c.

Monoclinic/orthogonal scanning. There exists only one orientation orbit and it contains just one orientation. When the c axis is chosen as the unique axis, the scanning group $\mathcal{H}$ is not only identical with the monoclinic space group $\mathcal{G}$ considered but it also has the same Hermann–Mauguin symbol. The vectors $\mathbf{a} = \mathbf{a}'$ and $\mathbf{b} = \mathbf{b}'$ of the monoclinic basis are taken as basis vectors of the lattices of sectional layer groups and the vector $\mathbf{c} = \mathbf{d}$ defines the scanning direction.

The Hermann–Mauguin symbol of the scanned group $\mathcal{G}$ changes with reference to a basis in which the b axis is chosen as

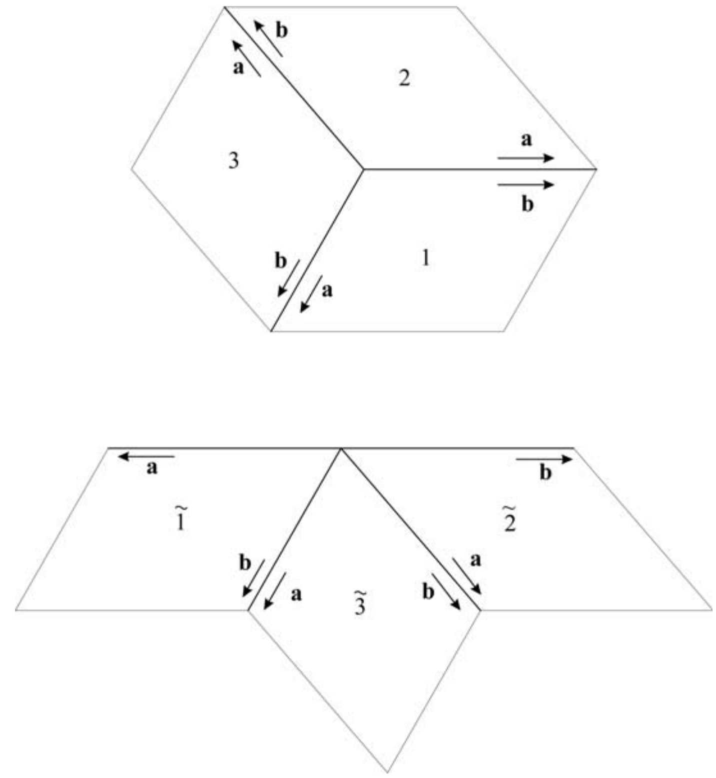

Fig. 5.2.4.1. Six monoclinic cell choices.

the unique axis. However, the Hermann–Mauguin symbol of the group in its role as the scanning group does not change, because the basis of the scanning group is chosen as $\mathbf{a}' = \mathbf{c}$, $\mathbf{b}' = \mathbf{a}$ and $\mathbf{d} = \mathbf{b}$.

Monoclinic/inclined scanning. There exists an infinite number of orientations for which the section planes are parallel with the unique axis. When the c axis is chosen as the unique axis, the orientations are specified by Miller indices ($mn0$). Each orientation orbit contains again just one orientation and the scanning group $\mathcal{H}$ is identical with the space group $\mathcal{G}$. The lattice of each sectional layer group is either a primitive or centred rectangular lattice with basis vectors $\mathbf{a}' = \mathbf{c}$ and $\mathbf{b}' = n\mathbf{a} - m\mathbf{b}$. The scanning direction is generally inclined to this orientation and the vector $\mathbf{d}$ can be chosen as any vector of the form $\mathbf{d} = p\mathbf{a} + q\mathbf{b}$, where p, q are integers that satisfy the condition $nq + mp = 1$ so that the vectors $\mathbf{a}'$, $\mathbf{b}'$ and $\mathbf{d}$ constitute a conventional unit cell of the scanning group, see Section 5.2.2.3.

The Hermann–Mauguin symbols for the group $\mathcal{H} = \mathcal{G}$ in its role as the scanning group are different to the symbol that specifies it as the scanned group because they refer to the choice of basis where the unique axis is defined by the vector $\mathbf{a}'$. The choice of the pair of vectors $\mathbf{b}' = n\mathbf{a} - m\mathbf{b}$ and $\mathbf{d} = p\mathbf{a} + q\mathbf{b}$ defines a cell choice to which the Hermann–Mauguin symbol of the group $\mathcal{H} = \mathcal{G}$ as the scanning group refers. Notice that the vector $\mathbf{b}'$ is defined by Miller indices ($mn0$) while freedom in the choice of the scanning direction $\mathbf{d}$ remains. The choice of vector $\mathbf{d}$ may influence the Hermann–Mauguin symbols of the scanning group and of the sectional layer groups but it does not change the groups.

When the b axis is chosen as the unique axis, the orientations of section planes are defined by Miller indices ($n0m$) and the conventional basis of the scanning group is chosen as $\mathbf{a}' = \mathbf{b}$, $\mathbf{b}' = n\mathbf{c} - m\mathbf{a}$, $\mathbf{d} = p\mathbf{c} + q\mathbf{a}$. The symbols of the group in its role as the scanning group for various parities of integers n, m, p and q, the linear orbits and the sectional layer groups are the same as in the case of unique axis c.

references