

5. SCANNING OF SPACE GROUPS

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 $(\hat{\mathbf{a}}, \hat{\mathbf{b}}, \hat{\mathbf{c}})$. 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 non-trivial 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 non-trivial 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 $\bar{1}$, $\bar{2}$, $\bar{3}$ 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

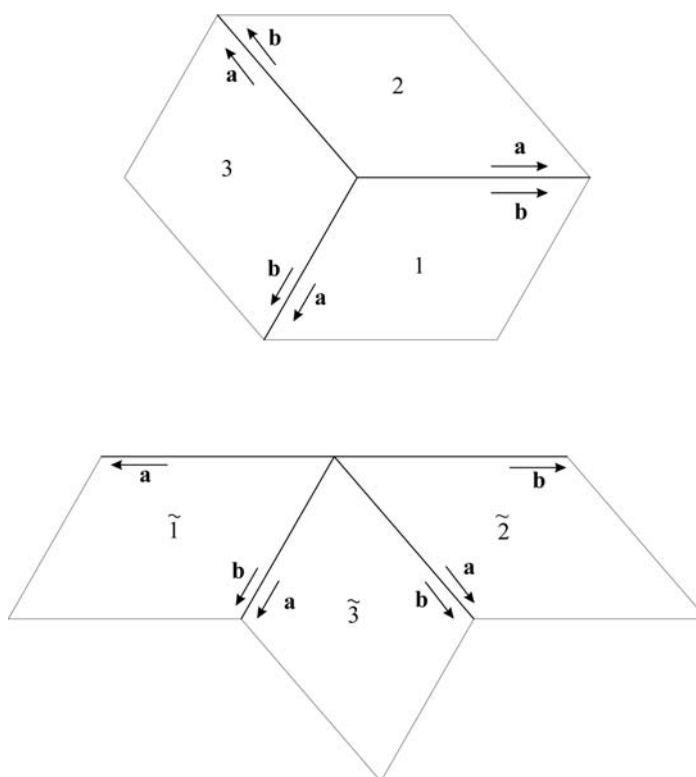


Fig. 5.2.4.1. Six monoclinic cell choices.

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 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

5.2. GUIDE TO THE USE OF THE SCANNING TABLES

q , the linear orbits and the sectional layer groups are the same as in the case of unique axis c .

The cases of monoclinic/inclined scanning appear in all groups of higher symmetries than monoclinic for those orientations for which the scanning group is monoclinic. These cases are collected in the auxiliary tables where reference to the monoclinic/inclined part of the monoclinic scanning tables is given in each particular case.

5.2.4.3. Orthorhombic system

All groups of the orthorhombic system belong to Laue class mmm (D_{2h}). The standard-format tables are given first for the geometric classes 222 (D_2), $mm2$ (C_{2v}) and mmm (D_{2h}). These are followed by the auxiliary tables.

5.2.4.3.1. Orthogonal scanning, standard tables

Orientation orbits (001), (100) and (010): These three orientation orbits represent all orbits with fixed parameters in the orthorhombic system. Each of these consists of a single orientation. Hence the scanning group \mathcal{H} for each of these orientations and for any orthorhombic group \mathcal{G} coincides with the group $\mathcal{G} = \mathcal{H}$ itself. The Hermann–Mauguin symbols of the scanning groups are, however, generally different for the three orientations because they refer to different bases \mathbf{a}' , \mathbf{b}' , $\mathbf{c}' = \mathbf{d}$. For the orientation (001) they always coincide with the Hermann–Mauguin symbol used in *IT A*.

The scanning groups for groups of geometric classes 222 (D_2) and mmm (D_{2h}) are not only the same (identical with the scanned group) for all three orientations, but in a few cases they also have the same Hermann–Mauguin symbols, so the entries in the columns of the scanning group and of the sectional layer groups coincide. The orbits are separated by horizontal lines in the first column and further through the column with the scanning group, orbits and sectional layer groups, if they are different; when the Hermann–Mauguin symbol of the scanning group and hence the two remaining columns are identical, we give them as a common row for all the three orbits, which are then separated only in the first two columns. In the tables for groups of geometric class $mm2$ (C_{2v}), the orbit (001) is separated by double lines across the table from the remaining orbits (100) and (010), which are separated by single lines across the tables.

The bases for the scanning groups and for the sectional layer groups associated with these orbits are chosen in a standard manner for all orthorhombic groups:

(1) For the orientation (001), it is natural to choose $\mathbf{a}' = \mathbf{a}$, $\mathbf{b}' = \mathbf{b}$ and $\mathbf{c}' = \mathbf{d} = \mathbf{c}$. The symbol of the scanning group then coincides with the symbol of the space group itself, *i.e.* its symbol in the (abc) setting.

(2) The scanning direction for orientations (100) and (010) are along $\mathbf{d} = \mathbf{a}$ and $\mathbf{d} = \mathbf{b}$, respectively. We choose the remaining vectors \mathbf{a}' , \mathbf{b}' in such a way that $(\mathbf{a}', \mathbf{b}', \mathbf{d})$ is a right-handed basis, hence $\mathbf{a}' = \mathbf{b}$, $\mathbf{b}' = \mathbf{c}$ for the orientation (100) and $\mathbf{a}' = \mathbf{c}$, $\mathbf{b}' = \mathbf{a}$ for the orientation (010). Accordingly, the Hermann–Mauguin symbols for the scanning groups are the symbols which correspond to the settings (bac) and $(\bar{c}ab)$, respectively.

5.2.4.3.2. Inclined scanning, auxiliary tables

Orientation orbits ($mn0$), ($0mn$) and ($n0m$): Each of these orientations has a scanning group of monoclinic symmetry, namely: 2 (C_2) for space groups of the geometric class 222 (D_2) in all settings and for the groups of the class $mm2$ (C_{2v}) in the (abc) setting; m (C_s) for groups of the geometric class $mm2$ (C_{2v}) in the settings (bac) , $(\bar{c}ab)$; and $2/m$ (C_{2h}) for groups of the geometric class mmm (D_{2h}) in all settings. In each case, the scanning group \mathcal{H} is a halving subgroup of the scanned group \mathcal{G} and consequently each orientation orbit contains two orientations with the same scanning group. The symmetry increases to orthorhombic and the

orbit contains one orientation for the special values $m = \pm 1$, $n = 0$ or $m = 0$, $n = \pm 1$.

The scanning groups are monoclinic and one can deduce them by viewing the diagrams of the scanned groups. By omitting the axes parallel with and planes perpendicular to the diagram plane, the diagram of the scanning group remains. This, however, is the diagram of the monoclinic scanning group in its standard setting when the unique axis is perpendicular to the plane of the diagram. This unique axis is a common direction for both orientations of the orbit and it is the c axis for the orientation orbit ($mn0$), and the a axis and b axis for the orientation orbits ($0mn$) and ($n0m$), respectively. The basis \mathbf{a}' , \mathbf{b}' , \mathbf{d} for the scanning group is expressed in the same way through the auxiliary basis and the scanning groups in the reference tables are given by their Hermann–Mauguin symbols with reference to the auxiliary bases. The three orbits are separated by horizontal lines in the tables of orientation orbits as well as in the first column of the reference tables. If the scanning group in a column for a certain scanned group \mathcal{G} has the same symbol for orbits in adjoining rows, we give it in a block common to these orbits.

Transformation of Miller indices for centred cases: In the table of orientation orbits for the C centring, we denote the orientation of the first orbit by $(hk0)$ and $(\bar{h}k0)$, *i.e.* we use letters h and k instead of m and n . The letters m and n are used for the Miller indices with respect to an auxiliary basis.

The scanning group is an equitranslational subgroup of the orthorhombic scanned group. Since the scanning group is monoclinic, the orthorhombic C lattice is considered as a monoclinic P lattice (with degenerate parameters) for which we choose the auxiliary basis vectors as $\hat{\mathbf{a}} = (\mathbf{a} - \mathbf{b})/2$, $\hat{\mathbf{b}} = (\mathbf{a} + \mathbf{b})/2$ and the unique axis vector $\hat{\mathbf{c}} = \mathbf{c}$.

The orientations are, however, defined by Miller indices $(hk0)$ with respect to the conventional basis $(\mathbf{a}, \mathbf{b}, \mathbf{c})$ of the orthorhombic group, while the numbers m, n define the Miller indices ($mn0$) with respect to the auxiliary basis $(\hat{\mathbf{a}}, \hat{\mathbf{b}}, \hat{\mathbf{c}})$. The scanning can be found at once from tables of scanning of monoclinic groups in terms of parities of m, n , and of p, q , where $\mathbf{b}' = n\hat{\mathbf{a}} - m\hat{\mathbf{b}}$ is determined by the orientation $(hk0)$ and p, q determine the scanning direction $\mathbf{d} = p\hat{\mathbf{a}} + q\hat{\mathbf{b}}$. Substituting for $\hat{\mathbf{a}}, \hat{\mathbf{b}}$ in vectors \mathbf{b}' and \mathbf{d} , we get

$$\hat{\mathbf{b}} = \frac{n-m}{2}\mathbf{a} - \frac{n+m}{2}\mathbf{b} = k\mathbf{a} - h\mathbf{b}, \quad (5.2.4.1)$$

so

$$k = \frac{n-m}{2}, \quad h = \frac{n+m}{2} \quad (5.2.4.2)$$

and conversely

$$n = h + k, \quad m = k - h. \quad (5.2.4.3)$$

If h is even and k odd, or h odd and k even, then both n and m are odd. However, if both h and k are odd (they cannot be simultaneously even), then both n and m are even, so that they cannot play the role of Miller indices, though they give the correct direction of the vector \mathbf{b}' . Dividing both by two, we get the Miller indices $(\frac{n}{2}\frac{m}{2}0)$ and either the case $\frac{n}{2}$ odd, $\frac{m}{2}$ even or the case $\frac{n}{2}$ even, $\frac{m}{2}$ odd may occur. Both $\frac{n}{2}$ and $\frac{m}{2}$ cannot be simultaneously either even or odd because in these cases both h and k will be even.

The same situation occurs for the orbit ($0mn$) of A -centred orthorhombic groups of the class $mm2$ (C_{2v}), where the vector \mathbf{a} plays the role of the unique monoclinic axis and for all three orientation orbits ($mn0$), ($0mn$) and ($n0m$) in the case of F -centred orthorhombic groups. In the latter case, the monoclinic scanning group is of the I -centred type with respect to the auxiliary bases while its centring in the bases $(\mathbf{a}', \mathbf{b}', \mathbf{d})$ depends on the choice of n, m (via h, k), and of p, q , see the monoclinic cases.