

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 $\bar{P}1$, 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 $\bar{P}1$, 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 $\bar{P}1$, 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

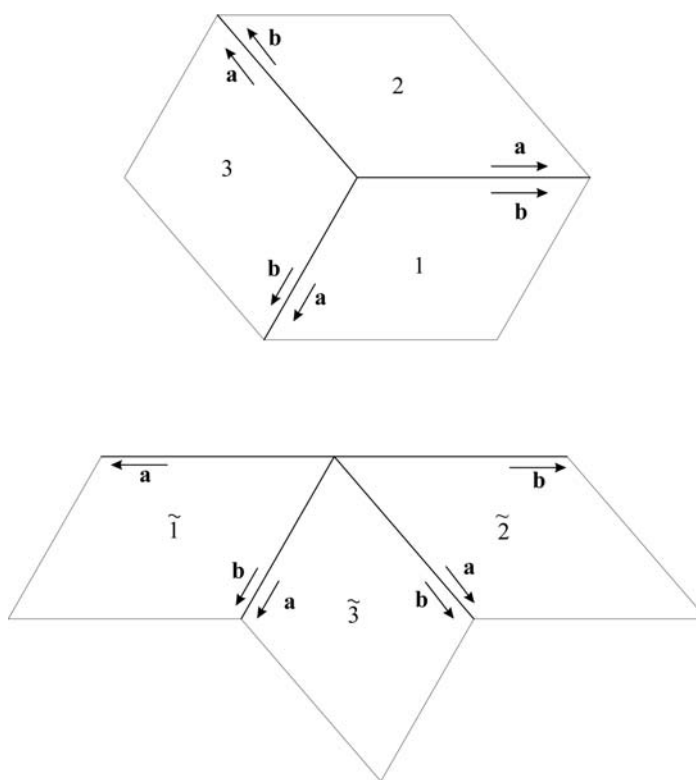


Fig. 5.2.4.1. Six monoclinic cell choices.

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