

5. SCANNING OF SPACE GROUPS

of the space group \mathcal{G} as well as of the scanning group \mathcal{H} in this interval. This length s_o is a fraction of unit interval, $s_o = \frac{1}{f}$, where $f = [H : L]$, $2[H : L]$ or $3[H : L]$ according to the centring of the scanning group and L is the point group of sectional layer groups corresponding to a general orbit.

5.2.2.7. Orthogonal, inclined and triclinic scanning

It is convenient for future reference to refine the basic categories of orthogonal and inclined scanning as follows:

(1) *Orthogonal scanning*. We call the scanning orthogonal if the scanning group is orthorhombic, tetragonal, trigonal or hexagonal.

(2a) *Monoclinic/orthogonal scanning*. This term is used if the scanning group is monoclinic and the vector \mathbf{d} defines its unique axis.

In both cases the vector \mathbf{d} is orthogonal to the vectors \mathbf{a}' and \mathbf{b}' and they occur whenever the orientation orbit is a special orbit with fixed parameters.

The absolute value $d = |\mathbf{d}|$ of the scanning vector is, in cases of orthogonal scanning, equal to the interplanar distance defined by the Miller indices of the orientation.

(2b) *Monoclinic/inclined scanning*. The scanning is called monoclinic/inclined if the scanning group is monoclinic and its unique axis is one of the vectors \mathbf{a}' , \mathbf{b}' . The vector \mathbf{d} is actually not necessarily inclined to the orientation $V(\mathbf{a}', \mathbf{b}')$. It may be orthogonal owing to special metric conditions of the lattice which are determined by the scanned group \mathcal{G} . It is, however, a vector of a monoclinic basis which lies in the plane orthogonal to the unique axis. This case occurs when the orientation orbit is a special orbit with one variable parameter.

The interplanar distance d in the case of inclined scanning is $d = |\mathbf{d}| \cos \varphi$ where φ is the angle of the vector \mathbf{d} with the normal to the plane.

(3) *Triclinic scanning*. The scanning is called triclinic or trivial if the scanning group is triclinic. This case occurs when the orientation orbit is a general orbit.

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.

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

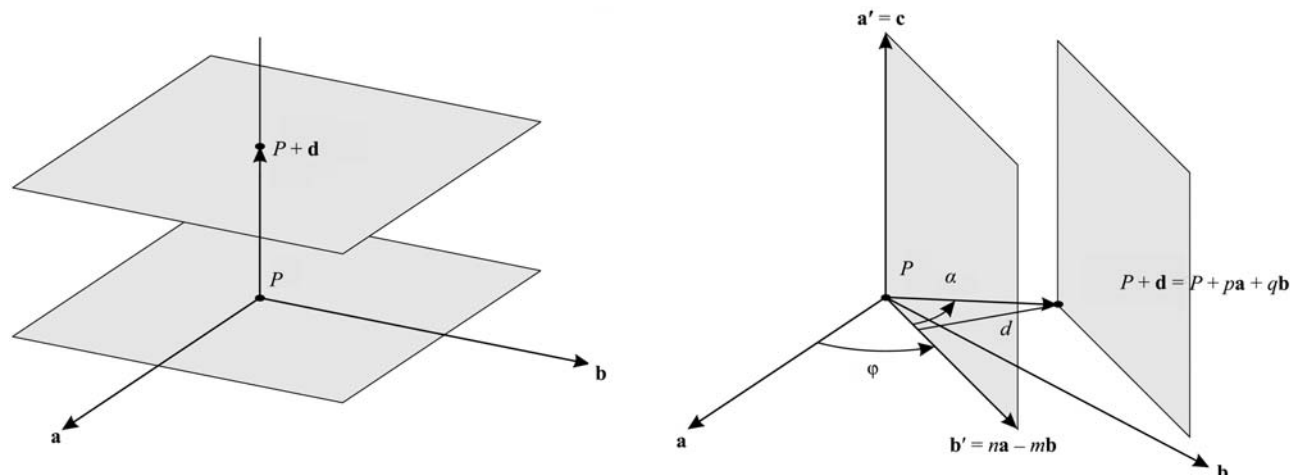


Fig. 5.2.2.2. Monoclinic/orthogonal (left) and monoclinic/inclined (right) scanning.