

5. SCANNING OF SPACE GROUPS

Whenever a transformation of Miller indices is used, it is printed in a special row across the table below the respective orbit; the transformation is the same for all three orbits in the case of F centring and is given once below the orbits.

5.2.4.4. Tetragonal system

The scanning in the tetragonal system has a slightly different character for groups of Laue class $4/m$ (C_{4h}) from those of Laue class $4/mmm$ (D_{4h}).

5.2.4.4.1. Orthogonal scanning, standard tables

Orientation orbit (001): This orbit with a single special orientation appears in all tetragonal groups. In each case, the tetragonal group itself is the scanning group for this orientation. For those tetragonal groups that are presented in *IT A* with two origin choices, we specify the scanning group by its Hermann–Mauguin symbol and origin choice in parentheses (usually below the symbol). The scanning groups are expressed with respect to bases identical with the original basis, so that the Hermann–Mauguin symbol of the scanning group is identical with the Hermann–Mauguin symbol of the scanned group including the origin choice, $\mathbf{a}' = \mathbf{a}$, $\mathbf{b}' = \mathbf{b}$ are the vectors of the conventional basis for the sectional layer groups and the scanning direction $\mathbf{d} = \mathbf{c}$ is along the main axis. In the same way, we will later refer to tetragonal scanning groups when performing the scanning of cubic groups. There are no other orientation orbits with fixed parameters for groups of classes 4 (C_4), $\bar{4}$ (S_4) and $4/m$ (C_{4h}), *i.e.* for the groups of Laue class $4/m$ (C_{4h}).

Orientation orbit (100): This orbit contains orientations (100) and (010); it appears in groups of geometric classes 422 (D_4), $4mm$ (C_{4v}), $\bar{4}2m$ (D_{2d}), and $4/mmm$ (D_{4h}), which belong to the Laue class $4/mmm$ (D_{4h}), but not in the groups of Laue class $4/m$ (C_{4h}). We choose the bases of scanning groups as $\mathbf{a}' = \mathbf{b}$, $\mathbf{b}' = \mathbf{c}$, $\mathbf{d} = \mathbf{a}$ for the orientation (100) and as $\mathbf{a}' = -\mathbf{a}$, $\mathbf{b}' = \mathbf{c}$, $\mathbf{d} = \mathbf{b}$ for the orientation (010). The corresponding scanning groups are orthorhombic and of the same centring type as the scanned group. In the majority of cases, the scanning groups are the same (*i.e.* expressed by the same Hermann–Mauguin symbol, with or without a shift) with respect to the two coordinate systems (P ; $\mathbf{a}' = \mathbf{b}$, $\mathbf{b}' = \mathbf{c}$, $\mathbf{d} = \mathbf{a}$) and (P ; $\mathbf{a}' = -\mathbf{a}$, $\mathbf{b}' = \mathbf{c}$, $\mathbf{d} = \mathbf{b}$) where P is the origin of the original group. In these cases, only one Hermann–Mauguin symbol (with or without a shift) is given for both orientations and one corresponding column of linear orbits and of sectional layer groups. Whenever this is not the case, the scanning group for one of the orientations is shifted with reference to its coordinate system as compared with the location of the other scanning group with reference to its coordinate system. There is also a respective shift of orientation orbits and of corresponding sectional layer groups. In these cases, the orientation-orbit row is split into two parts, each referring to one orientation of the orbit.

Orientation orbit (110): The orbit contains the orientations (110) and ($\bar{1}\bar{1}0$); it again appears in all groups of the geometric classes 422 (D_4), $4mm$ (C_{4v}), $\bar{4}2m$ (D_{2d}) and $4/mmm$ (D_{4h}) belonging to the Laue class $4/mmm$ (D_{4h}), but not in the groups of Laue class $4/m$ (C_{4h}). We choose the bases of scanning groups as $\mathbf{a}' = (-\mathbf{a} + \mathbf{b})$, $\mathbf{b}' = \mathbf{c}$, $\mathbf{d} = (\mathbf{a} + \mathbf{b})$ for the orientation (110) and as $\mathbf{a}' = (\mathbf{a} + \mathbf{b})$, $\mathbf{b}' = \mathbf{c}$, $\mathbf{d} = (\mathbf{a} - \mathbf{b})$ for the orientation ($\bar{1}\bar{1}0$). The resulting scanning groups are again orthorhombic of centring type C (denoted by B in view of the choice of the basis) when the original tetragonal group is of the type P and of centring type F when the original tetragonal group is of the type I . The scanning group, respective linear orbits and sectional layer groups are either the same with reference to the coordinate systems (P ; $\mathbf{a}' = (-\mathbf{a} + \mathbf{b})$, $\mathbf{b}' = \mathbf{c}$, $\mathbf{d} = (\mathbf{a} + \mathbf{b})$) and (P ; $\mathbf{a}' = (\mathbf{a} + \mathbf{b})$, $\mathbf{b}' = \mathbf{c}$, $\mathbf{d} = (\mathbf{a} - \mathbf{b})$) or one of them is shifted with respect to the other. Accordingly, the row for the orbit either does not split or it splits into two subrows for the two orientations.

5.2.4.4.2. Inclined scanning, auxiliary tables

Orientation orbits ($mn0$) occur in groups of both tetragonal Laue classes $4/m$ (C_{4h}) and $4/mmm$ (D_{4h}). Orientation orbits ($0mn$) occur only in groups of the Laue class $4/mmm$ (D_{4h}).

Orientation orbits ($mn0$): These orbits contain two orientations, namely ($mn0$) and ($\bar{n}m0$) in groups of the geometric classes 4 (C_4), $\bar{4}$ (S_4) and $4/m$ (C_{4h}) which belong to the Laue class $4/m$ (C_{4h}), and four orientations, namely ($mn0$), ($\bar{n}m0$), ($\bar{m}n0$) and ($n\bar{m}0$) in groups of the geometric classes 422 (D_4), $4mm$ (C_{4v}), $\bar{4}2m$ (D_{2d}) and $4/mmm$ (D_{4h}) which belong to the Laue class $4/mmm$ (D_{4h}).

For special values $m = 1$ and $n = 0$, the orbit contains only two orientations (100) and (010) which form an orbit with fixed parameters with an orthorhombic scanning group for groups of the Laue class $4/mmm$ (D_{4h}). For groups of the Laue class $4/m$ (C_{4h}) these two orientations represent just one particular case of the orbit ($mn0$). Analogously, the orbit with two orientations (110) and ($\bar{1}\bar{1}0$) for groups of the Laue class $4/mmm$ (D_{4h}) is an orbit with fixed parameters $m = 1$, $n = 1$ while for groups of the Laue class $4/m$ (C_{4h}) it is a particular case of the orbits ($mn0$).

There are no other special orbits with variable parameter in groups of the Laue class $4/m$ (C_{4h}). Auxiliary bases are defined by one table common for both centring types P and I .

Auxiliary bases for this orbit are also common for both centring types in groups of the Laue class $4/mmm$ (D_{4h}) and they are given in the tables of orientation orbits for both types.

Orientation orbits ($0mn$): These orbits, consisting of orientations ($0mn$), ($0\bar{m}n$), ($m0n$) and ($m0\bar{n}$), appear only in groups of the Laue class $4/mmm$ (D_{4h}). The first two orientations contain the vector \mathbf{a} , the other two contain the vector \mathbf{b} , scanning groups are monoclinic with unique axes along vectors \mathbf{a} and \mathbf{b} , respectively, for the first and second pair of orientations; the scanning is inclined because the vectors \mathbf{a} and \mathbf{b} lie in the respective orientations. To primitive and centred lattices of the scanned groups there correspond primitive and centred lattices of the scanning groups, respectively, which is reflected in the reference tables.

Auxiliary bases for this orbit are common for both centring types in groups of the Laue class $4/mmm$ (D_{4h}) and they are given in tables of orientation orbits for both types.

For special values of parameters, the orbit coincides either with the orbit (100), (010) or with the orbit (110), ($\bar{1}\bar{1}0$).

Orientation orbits (hhl): These orbits, consisting of orientations (hhl), ($\bar{h}\bar{h}l$), ($h\bar{h}l$) and ($\bar{h}hl$), appear again only in groups of the Laue class $4/mmm$ (D_{4h}). The first two orientations contain the vector $(\mathbf{a} - \mathbf{b})$, the other two contain the vector $(\mathbf{a} + \mathbf{b})$, scanning groups are monoclinic with unique axes along these vectors $(\mathbf{a} - \mathbf{b})$ and $(\mathbf{a} + \mathbf{b})$, respectively, for the first and second pair of orientations; the scanning is again inclined because the vectors $(\mathbf{a} - \mathbf{b})$ and $(\mathbf{a} + \mathbf{b})$ lie in the respective orientations.

The auxiliary bases for the monoclinic scanning groups in the case of a primitive (P) tetragonal lattice are chosen as

$$\hat{\mathbf{a}} = \mathbf{a} + \mathbf{b}, \quad \hat{\mathbf{b}} = \mathbf{c} \quad \text{and} \quad \hat{\mathbf{c}} = \mathbf{a} - \mathbf{b} \quad (5.2.4.4)$$

for the first pair of orientations and as

$$\hat{\mathbf{a}} = \mathbf{b} - \mathbf{a}, \quad \hat{\mathbf{b}} = \mathbf{c} \quad \text{and} \quad \hat{\mathbf{c}} = \mathbf{a} + \mathbf{b} \quad (5.2.4.5)$$

for the second pair of orientations.

The auxiliary bases for the monoclinic scanning groups in the case of an I -centred tetragonal lattice are chosen as

$$\hat{\mathbf{a}} = (\mathbf{a} + \mathbf{b} + \mathbf{c})/2, \quad \hat{\mathbf{b}} = \mathbf{c} \quad \text{and} \quad \hat{\mathbf{c}} = (\mathbf{a} - \mathbf{b}) \quad (5.2.4.6)$$

for the first pair of orientations and as

$$\hat{\mathbf{a}} = (\mathbf{b} - \mathbf{a} + \mathbf{c})/2, \quad \hat{\mathbf{b}} = \mathbf{c} \quad \text{and} \quad \hat{\mathbf{c}} = (\mathbf{a} + \mathbf{b}) \quad (5.2.4.7)$$

for the second pair of orientations.

A vector parallel with planes of orientation (hhl) and orthogonal to $\mathbf{a} - \mathbf{b}$ is a multiple of