International Tables for Crystallography (2006). Vol. E, Section 5.2.4.4.2, pp. 404–405.

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}), $\bar{4}2m$ or $\bar{4}m2$ (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 ($1\bar{1}0$); 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 ($1\bar{1}0$). 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 ($nm0$) 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 ($1\bar{1}0$) 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), ($1\bar{1}0$).

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

$$\widehat{\mathbf{a}} = \mathbf{a} + \mathbf{b}, \quad \widehat{\mathbf{b}} = \mathbf{c} \quad \text{and} \quad \widehat{\mathbf{c}} = \mathbf{a} - \mathbf{b} \tag{5.2.4.4}$$

for the first pair of orientations and as

$$\widehat{\mathbf{a}} = \mathbf{b} - \mathbf{a}, \quad \widehat{\mathbf{b}} = \mathbf{c} \quad \text{and} \quad \widehat{\mathbf{c}} = \mathbf{a} + \mathbf{b} \tag{5.2.4.5}$$

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

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

for the first pair of orientations and as

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

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

$$2h\mathbf{c} - l(\mathbf{a}+\mathbf{b}). \qquad (5.2.4.8)$$

In terms of Miller indices $(mn0)$ with reference to the first auxiliary basis for a P-centred lattice, such a vector is a multiple of

$$m\mathbf{c} - n(\mathbf{a}+\mathbf{b}) \qquad (5.2.4.9)$$

and in terms of Miller indices $(mn0)$ with reference to the first auxiliary basis for an I-centred lattice, it is a multiple of

$$(2m-n)\mathbf{c} - n(\mathbf{a}+\mathbf{b}). \qquad (5.2.4.10)$$

Therefore, for a P-centred lattice, the pair of numbers (m, n) must be proportional to the pair $(2h, l)$. Since Miller indices must be relatively prime, we get $n = l$, $m = 2h$ if l is odd and $n = l/2$, $m = h$ if l is even.

For an I-centred lattice, the pair of numbers $(2m-n, n)$ must be proportional to the pair $(2h, l)$ and hence the pair $(2m, n)$ must be proportional to the pair $(2h+l, l)$. If l is odd, then $2h+l$ is also odd and we put $m = 2h+l$, so that $n = 2l$. If l is even, we put $n = l$ and $m = h + l/2$.

These relations are printed in the last rows across the tables of orientation orbits within the block for orbit (hhl).

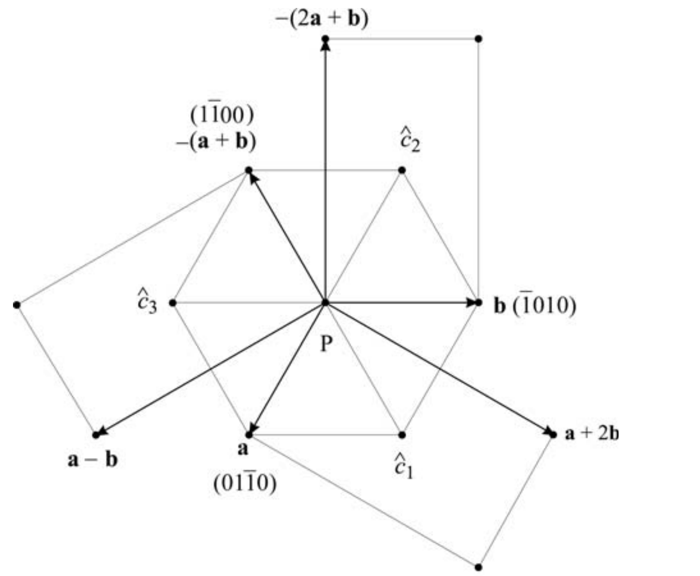

Fig. 5.2.4.2. Symbols for a hexagonal lattice with a rectangular point group.

5.2.4.5. *Hexagonal family*

The family splits into the trigonal and the hexagonal system. With the exception of seven group types with rhombohedral lattices [$R3$, C_3^4 (No. 146); $R\bar{3}$, C_{3i}^2 (No. 148); $R32$, D_3^7 (No. 155); $R3m$, C_{3v}^5 (No. 160); $R3c$, C_{3v}^6 (No. 161); $R\bar{3}m$, D_{3d}^5 (No. 166); and $R\bar{3}c$, D_{3d}^6 (No. 167)] all space groups of both systems have a primitive hexagonal lattice. Scanning tables are given in the hexagonal coordinate system for all groups with this lattice and the bases of the scanning groups for individual orientations are chosen identically. For the seven groups with rhombohedral lattices, the description of scanning in the hexagonal coordinate system differs from the description in the rhombohedral coordinate system only in the specification of orientations by Bravais–Miller and Miller indices, respectively. The column *Orientation orbit* is split into two columns with the headings Hexag. axes and Rhomb. axes.

5.2.4.5.1. *Orthogonal scanning, standard tables*

Orientation orbit (0001): The orientation (0001) is invariant under all point groups of the family; it forms therefore an orientation orbit with a single special orientation in all space groups of the family and the scanning groups for this orientation coincide with the scanned groups. We choose $\mathbf{a}' = \mathbf{a}$, $\mathbf{b}' = \mathbf{b}$, $\mathbf{d} = \mathbf{c}$ in primitive as well as in rhombohedral cases; in the latter case, the orientation is also specified in the second column as (111). The Hermann–Mauguin symbols of the scanning groups also coincide with the symbols of the scanned groups; to specify both the scanned and the scanning groups with rhombohedral lattices with reference to hexagonal bases we use an obverse setting as in *IT* A.

All corresponding sectional layer groups have the same planar hexagonal lattice with basis vectors $\mathbf{a}' = \mathbf{a}$ and $\mathbf{b}' = \mathbf{b}$. The basis $(\mathbf{a}, \mathbf{b})$, denoted as usual by p, is the conventional basis for all trigonal/hexagonal, hexagonal/hexagonal, monoclinic/oblique and triclinic/oblique sectional layer groups. To describe the monoclinic/rectangular and orthorhombic/rectangular sectional layer groups, we choose three conventional rectangular bases: $\widehat{c}_1 = (\mathbf{a}, \mathbf{a}+2\mathbf{b})$, $\widehat{c}_2 = (\mathbf{b}, -(2\mathbf{a}+\mathbf{b}))$ and $\widehat{c}_3 = (-(\mathbf{a}+\mathbf{b}), (\mathbf{a}-\mathbf{b}))$, as shown in Fig. 5.2.4.2. The symbols $\widehat{c}_1, \widehat{c}_2, \widehat{c}_3$ then denote the same lattice, identical with the p-lattice with the conventional basis $(\mathbf{a}, \mathbf{b})$.

In the cases of the trigonal space-group types $P3_112$, D_3^3 (No. 151), $P3_121$, D_3^4 (No. 152), $P3_212$, D_3^5 (No. 153) and $P3_221$, D_3^6 (No. 154), and in the cases of the hexagonal space-group types $P6_122$, D_6^2 (No. 178) and $P6_522$, D_6^3 (No. 179), there exist two linear orbits with fixed parameter for which the sectional layer groups are monoclinic/rectangular with a c-centred lattice. The orientations of the unique axes of the respective monoclinic/rectangular groups are then defined by the choice of the conventional basis to which the Hermann–Mauguin symbol refers (*i.e.* by index in $\widehat{c}_1$, $\widehat{c}_2$ or $\widehat{c}_3$) and by the position of the twofold rotation in the symbol. In group types $P6_222$, D_6^4 (No. 180) and $P6_422$, D_6^5 (No. 181) there exist two linear orbits with fixed parameters for which the sectional layer groups are orthorhombic/rectangular with a c-centred lattice. The orientations of twofold axes of orthorhombic/rectangular groups in the section plane are again defined by the conventional bases $\widehat{c}_1$, $\widehat{c}_2$ or $\widehat{c}_3$. There are no other non-trivial orientation orbits in groups of the Laue class $\bar{3}$ (C_{3i}) and no other orbits with fixed parameters in groups of the Laue class $6/m$ (C_{6h}).

Orientation orbits $(01\bar{1}0)$ *and* $(\bar{1}2\bar{1}0)$: These two orbits appear in all biaxial groups of the trigonal and hexagonal system, *i.e.* in groups of the Laue classes $\bar{3}m$ (D_{3d}) and $6/mmm$ (D_{6h}). We consider them together because corresponding scanning groups for pairs of orientations, one from each of these orbits, are related in the same way to their corresponding bases.

Hexagonal lattice. If the scanned group is trigonal with a primitive hexagonal lattice, the scanning group is monoclinic; if

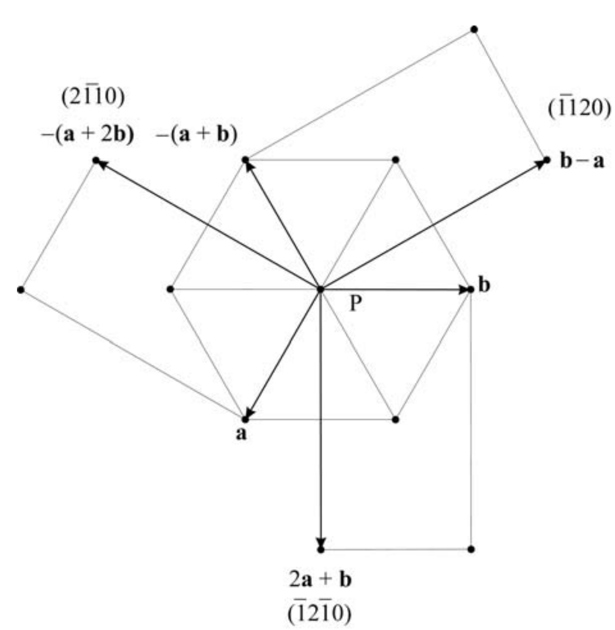

Fig. 5.2.4.3. Another choice of orthogonal basis vectors for a hexagonal lattice.

references