*International Tables for Crystallography* (2010). Vol. B, Section 1.5.5.4.4, pp. 190–191.



three of them do not appear and the length of the others depends on the boundary plane, see Tables and Figs. 1.5.5.5 to 1.5.5.7.

The boundary conditions for the asymmetric unit are independent of the lattice parameters and the boundary plane is always represented by the simple equation $x, y, \frac{1}{2}$: $0 < x, y < \frac{1}{2}$. By introducing flagpoles and wings, the description may become uni-arm.

#### 1.5.5.4.2. *Splitting of k-vector types*

The Brillouin zone as well as the unit cell are always convex bodies; the same holds for the representation domain of CDML and for the choice of the asymmetric unit. It is thus sometimes unavoidable that the **k**-vector types are split and that the different parts belong to different arms and to different stars of **k** vectors. Sometimes this splitting of **k**-vector types may be avoided by an appropriate choice of the asymmetric unit; sometimes the introduction of flagpoles and wings is necessary to make the **k**-vector types uni-arm.

*Examples*

(1) In the reciprocal-space group $(\mathcal{G})^* = (Fm\overline{3}m)^*$, No. 225 of the arithmetic crystal class $m\overline{3}mI$ there are the lines of **k** vectors $\Lambda$ $(\alpha, \alpha, \alpha)$ and $F$ $(\frac{1}{2} - \alpha, -\frac{1}{2} + 3\alpha, \frac{1}{2} - \alpha)$ of CDML, p. 41. By Figure 1.5.5.1 one sees that the line $\Lambda$ connects the points $\Gamma$ and $P$, the line $F$ connects the points $P$ and $H$. One takes from the corresponding Table 1.5.5.1 the coefficients of $P = \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ and $H = 0, \frac{1}{2}, 0$. From these points or from the transformation listed at the top of Table 1.5.5.1 as 'Parameter relations' the coefficients of the line $F$ are obtained as $F = x, \frac{1}{2} - x, x$; $0 < x < \frac{1}{4}$.

The inspection of the symmetry diagram of $Fm\overline{3}m$, No. 225, in *IT* A shows that a twofold rotation 2 (represented by the $4_2$ $\frac{1}{4}, y, \frac{1}{4}$ screw-rotation axis) leaves the point $P$ invariant, whereas the point $H$ is mapped onto the point $R$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$. More formally: the rotation is described by $x, \frac{1}{2} - x, x \rightarrow \frac{1}{2} - x, \frac{1}{2} - x, \frac{1}{2} - x$, where $0 < x < \frac{1}{4}$. The result is the line $F_1 = [R\,P]$. It is uni-arm to the line $\Lambda = x, x, x$ and the union $\Lambda \cup F_1$ forms the Wintgen position 32 $f$ $3m$. An analogous result is obtained for the same lines in the arithmetic crystal class $m\overline{3}I$.

(2) In the following example the splitting of a Wintgen position happens if a representation domain of the Brillouin zone is chosen. The splitting can be avoided by the choice of the asymmetric unit. We consider the plane $x, y, 0$ in the arithmetic crystal class $4/mmmI$, see Fig. 1.5.5.4 and Table 1.5.5.4. In CDML this plane is split into the parts $C = [\Gamma\,S_2\,R\,X]$ and $D = [M\,S\,G] \sim [M_2\,S_2\,R]$. By the choice of the asymmetric unit the independent region of the Wintgen position is uni-arm: $[\Gamma M_2 X] = 16$ $l$ $m..$ $x, y, 0$: $0 < x < y < \frac{1}{2}$.

(3) The splitting of a Wintgen position can be avoided if flagpoles and wings are admitted, *i.e.* if the minimal domain is described by a non-convex body. If one chooses in the first example of the arithmetic crystal classes $m\overline{3}mI$ and $m\overline{3}I$ the union $\Lambda \cup F_1$ for the line $x, x, x$, then $F_1 = [P\,R]$ forms a flagpole, whereas $\Lambda$ forms an edge of the asymmetric unit, see Figs. 1.5.5.1 and 1.5.5.2.

The same holds for the Wintgen position 96 $k$ $..m$ $x, x, z$ of $m\overline{3}mI$. In the representation domain which is simultaneously the asymmetric unit, this Wintgen position is split into three parts $B$, $C$ and $J$, which form three of the four walls of the (tetrahedral) minimal domain. By proper symmetry operations these three parts can be made uni-arm to the part $C$, such that their union $C \cup B_1 \cup J_1$ describes the independent part of that Wintgen position, see Fig. 1.5.5.1. The part $C$ forms a wall of the asymmetric unit; the part $B_1 \cup J_1$ forms a wing, see Fig. 1.5.5.1.

#### 1.5.5.4.3. *k-vector types for non-holosymmetric space groups*

The **k**-vector labels of CDML are primarily listed for the holosymmetric space groups. These lists are kept and supplemented for the non-holosymmetric space groups. In this way many superfluous **k**-vector labels are introduced.

*Examples*

(1) Arithmetic crystal class $m\overline{3}I$. In its reciprocal-space group $(Fm\overline{3})^*$, the introduction of the plane $AA = [\Gamma\,H_2\,N]$ is unnecessary because the plane $A = [\Gamma\,N\,H]$ of Wintgen position 96 $j$ $m..$ of $(Fm\overline{3}m)^*$ can be extended to $A \cup AA = [\Gamma\,H_2\,H]$ in the reciprocal-space group $(Fm\overline{3})^*$, *cf.* Fig. 1.5.5.2 and Table 1.5.5.2. In $(Fm\overline{3})^*$, both planes, $A$ and $AA$, belong to Wintgen position 48 $h$ $m..$. The parameter description is extended from $x, y, 0$: $0 < x < y < \frac{1}{2} - x (< \frac{1}{4})$ to $0 < y < \frac{1}{2} - x < \frac{1}{2}$.

(2) In the previous example, during the transition from the group $(Fm\overline{3}m)^*$ to the subgroup $(Fm\overline{3})^*$ the order of the little co-group of the special **k** vectors of $(Fm\overline{3}m)^*$ was not changed. In other cases, the little co-group may be reduced to a subgroup. Such **k** vectors may then be incorporated into a more general Wintgen position and described by an extension of the parameter range.

Arithmetic crystal class $m\overline{3}mI$, plane $[\Gamma\,H\,N] = x, y, 0$. In $(Fm\overline{3}m)^*$, see Fig. 1.5.5.1, all points ($\Gamma$, $H$, $N$) and lines ($\Delta$, $\Sigma$, $G$) of the boundary of the asymmetric unit are special. In $(Fm\overline{3})^*$, see Fig. 1.5.5.2, the lines $\Delta$ and $[\Gamma\,H_2] \sim \Delta$ are special but $\Sigma$, $G$ and $[N\,H_2] \sim G$ belong to the plane $(A \cup AA)$. The free parameter range on the line $G$ is $0 < y < \frac{1}{4}$. Therefore, the parameter ranges of $(A \cup AA \cup G \cup \Sigma)$ in $x, y, 0$ can be taken as: $0 < x < \frac{1}{2} - y < \frac{1}{2}$ for $A \cup AA \cup \Sigma$ and $0 < y = \frac{1}{2} - x < \frac{1}{4}$ for $G$.

#### 1.5.5.4.4. *Ranges of independent parameters*

In Section 1.5.4.3 a method for the determination of the parameter ranges was described. A few examples shall display the procedure.

(1) Arithmetic crystal class $m\overline{3}mI$, line $\Lambda \cup F_1$: In the reciprocal-space group $(Fm\overline{3}m)^*$ of the arithmetic crystal class $m\overline{3}mI$, the line $x, x, x$ has stabilizer $\overline{3}m$ and little co-group $\overline{\mathcal{G}}^{\mathbf{k}} = 3m$. Therefore, the divisor is 12:6 = 2 and $x$ is running from 0 to $\frac{1}{2}$.

The same result holds for the line $\Lambda \cup F_1$ in the reciprocal-space group $(Fm\overline{3})^*$ of the arithmetic crystal class $m\overline{3}I$: the stabilizer generated by $\overline{3}$ is of order 6, $|\overline{\mathcal{G}}^{\mathbf{k}}| = |\{3\}| = 3$, the quotient is again $\frac{1}{2}$, the parameter range is the same as for $(Fm\overline{3}m)^*$.

(2) Arithmetic crystal class $m\overline{3}mI$, plane $B_1 \cup C \cup J_1$: In $(Fm\overline{3}m)^*$, the stabilizer of $x, x, z$ is generated by $m.mm$ and the centring translation $t(\frac{1}{2}, \frac{1}{2}, 0)$ mod (integer translations). They generate a group of order 16; $\overline{\mathcal{G}}^{\mathbf{k}}$ is $..m$ of order 2. The fraction of the plane is $\frac{2}{16} = \frac{1}{8}$ of the area $\sqrt{2}a^{*2}$ in the (centred) unit cell, as expressed by the parameter ranges $0 < x < \frac{1}{4}, 0 < z < \frac{1}{2}$. There are six arms of the star of $x, x, z$: $x, x, z$; $\overline{x}, x, z$; $x, y, x$; $x, y, \overline{x}$; $x, y, y$; $x, \overline{y}, y$. Three of them ($x, x, z$, $\overline{x}, x, z$ and $x, y, x$) are represented in the boundaries of the representation domain: $C = [\Gamma\,N\,P]$, $B = [H\,N\,P]$ and $J = [\Gamma\,H\,P]$, see Fig. 1.5.5.1. The areas of their parameter ranges are $\frac{1}{32}, \frac{1}{32}$ and $\frac{1}{16}$, respectively; the sum is $\frac{1}{8}$.

Arithmetic crystal class $m\overline{3}I$, the same result holds in the reciprocal-space group $(Fm\overline{3})^*$. The stabilizer generated by $2/m..$ and by the centring translation $t(\frac{1}{2}, \frac{1}{2}, 0)$ mod (integer translations) forms a group of order 8; the order of the little co-group $|\overline{\mathcal{G}}^{\mathbf{k}}| = |\{1\}| = 1$. The quotient is again $\frac{1}{8}$, the parameter range is the same as for $(Fm\overline{3}m)^*$ but the plane belongs to the general position *GP* because the little co-group is trivial.

(3) Arithmetic crystal class $m\overline{3}mI$, reciprocal-space group $(Fm\overline{3}m)^*$, plane $x, y, 0$: the stabilizer of the plane $A$ is generated by $4/mmm$ and $t(\frac{1}{2}, \frac{1}{2}, 0)$, order 32, $\overline{\mathcal{G}}^{\mathbf{k}}$ (site-symmetry group) $m..$,

order 2. Consequently, $[\Gamma\ H\ N]$ is $\frac{1}{16}$ of the unit square $a^{*2}$: $0 < x < y < \frac{1}{2} - x$. In $(Fm\overline{3})^*$, the stabilizer of $x, y, 0$, here $A \cup AA$, is *mmm*. and $t(\frac{1}{2}, \frac{1}{2}, 0)$, order 16, with the same group $\overline{\mathcal{G}}^{\mathbf{k}} = m..$ of order 2. Therefore, $[\Gamma\ H_2\ H]$ is $\frac{1}{8}$ of the unit square $a^{*2}$ in $(Fm\overline{3})^*$; $0 < y < \frac{1}{2} - x < \frac{1}{2}$.

(4) Arithmetic crystal class $m\overline{3}mI$, line $x, x, 0$: In $(Fm\overline{3}m)^*$ the stabilizer is generated by $m.mm$ and $t(\frac{1}{2}, \frac{1}{2}, 0)$ mod (integer translations), order 16, $\overline{\mathcal{G}}^{\mathbf{k}}$ is $m.2m$ of order 4. The divisor is 4 and thus $0 < x < \frac{1}{4}$. In $(Fm\overline{3})^*$ the stabilizer is generated by $2/m..$ and $t(\frac{1}{2}, \frac{1}{2}, 0)$ mod (integer translations), order 8, and $\overline{\mathcal{G}}^{\mathbf{k}} = m..$, order 2; the divisor is 4 again and $0 < x < \frac{1}{4}$ is restricted to the same range.

In the way just described the *inner* part of the parameter range can be fixed. The *boundaries* of the parameter range must be determined in addition:

(1) Arithmetic crystal classes $m\overline{3}mI$ and $m\overline{3}I$, *i.e.* $(Fm\overline{3}m)^*$ and $(Fm\overline{3})^*$, line $x, x, x$: The points $0, 0, 0$; $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ (and $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$) are special points; the parameter ranges are open: $0 < x < \frac{1}{4}$, $\frac{1}{4} < x < \frac{1}{2}$.

(2) Arithmetic crystal class $m\overline{3}mI$, plane $x, x, z$: In $(Fm\overline{3}m)^*$ all corners $\Gamma$, $N$, $N_2$, $H_2$ and all edges are special points or lines. Therefore, the parameter ranges are open: $x, x, z$: $0 < x < \frac{1}{4}, 0 < z < \frac{1}{2}$, where the lines $x, x, x$: $0 < x < \frac{1}{4}$ and $x, x, \frac{1}{2} - x$: $0 < x < \frac{1}{4}$ are special lines and thus excepted.

(3) Arithmetic crystal classes $m\overline{3}mI$ and $m\overline{3}I$, plane $x, y, 0$: In both reciprocal-space groups, $(Fm\overline{3}m)^*$ and $(Fm\overline{3})^*$, $0 < x$ and $0 < y$ holds. The line $0, y, 0 = \Delta$ is a special line, its $\mathbf{k}$ vectors have little co-groups of higher order than that of the planes $x, y, 0$ and the boundaries of both planes are open. The same holds for the boundary $x, 0, 0 \sim 0, y, 0$ for $(Fm\overline{3})^*$. The $\mathbf{k}$ vectors of the lines $x, x, 0$ and $x, \frac{1}{2} - x, 0$, $\Sigma$ and $G$, also have little co-groups of higher order and belong to other Wintgen positions in the representation domain (or asymmetric unit) of $(Fm\overline{3}m)^*$. Therefore, for the arithmetic crystal class $m\overline{3}mI$, the plane $A = x, y, 0$ is open at its boundaries $x, x, 0$ and $x, \frac{1}{2} - x, 0$ in the range $0 < x < \frac{1}{4}$. In the asymmetric unit of $(Fm\overline{3})^*$ the lines $x, x, 0$: $0 < x < \frac{1}{4}$ and $x, \frac{1}{2} - x, 0$: $0 < x < \frac{1}{4}$ belong to the plane, and the boundary of the plane $A$ is here closed. The boundary line $x, \frac{1}{2} - x, 0$: $\frac{1}{4} < x < \frac{1}{2}$ of the plane $AA$ is equivalent to the range $0 < x < \frac{1}{4}$ of the part $A$ and thus does not belong to the asymmetric unit; here the boundary of the plane $A \cup AA$ is open.

Data on the independent parameter ranges are essential to make sure that exactly one $\mathbf{k}$ vector per orbit is represented in the representation domain $\Phi$ or in the asymmetric unit. Such data are often much easier to calculate for the asymmetric unit of the unit cell than for the representation domain of the Brillouin zone, in particular if a uni-arm description has been chosen, *cf.* Section 1.5.5. Such data can not be found in the cited tables of irreps.

The uni-arm description unmasks those $\mathbf{k}$ vectors which lie on the boundary of the Brillouin zone but belong to a Wintgen position which also contains inner $\mathbf{k}$ vectors, see the example of the lines $\Lambda$ and $F$ in $(Fm\overline{3}m)^*$ and $(Fm\overline{3})^*$. Such $\mathbf{k}$ vectors can not give rise to little-group representations obtained from projective representations of the little co-group $\overline{\mathcal{G}}^{\mathbf{k}}$.

The consideration of the basic domain $\Omega$ in relation to the representation domain $\Phi$ is unnecessary. It may even be misleading because special $\mathbf{k}$-vector subspaces of $\Omega$ frequently belong to more general types of $\mathbf{k}$ vectors in $\Phi$. Space groups $\mathcal{G}$ with non-holohedral point groups can be referred to their reciprocal-space groups $(\mathcal{G})^*$ directly without reference to the types of irreps of the corresponding holosymmetric space group.

In principle both approaches are equivalent: the *traditional* one by Brillouin zone, basic domain and representation domain and the *crystallographic* one by unit cell and asymmetric unit. Moreover, it is not difficult to relate one approach to the other, see Figs. and Tables 1.5.5.1 to 1.5.5.7. The conclusions show that the crystallographic approach for the description of irreps of space groups has several advantages as compared with the traditional approach. Owing to these advantages, CDML have already accepted the crystallographic approach for triclinic and monoclinic space groups. However, the advantages are not restricted to such low symmetries. In particular, the simple boundary conditions and shapes of the asymmetric units result in simple equations for the boundaries and shapes of volume elements and facilitate numerical calculations, integrations *etc.* If there are special reasons to prefer $\mathbf{k}$ vectors inside or on the boundary of the Brillouin zone to those outside, then the advantages and disadvantages of both approaches have to be compared in order to find the optimal way to solve the problem.

The crystallographic approach may be realized in three different ways:

(1) In the *uni-arm description* one lists each $\mathbf{k}$-vector star exactly once by indicating the parameter field of the representing $\mathbf{k}$ vector. Advantages are the transparency of the presentation and the relatively small effort for the derivation of the list. A disadvantage may be that there are protruding flagpoles or wings. Points of flagpoles or wings are no longer neighbours of inner points (an inner point has a full three-dimensional sphere of neighbours which belong to the asymmetric unit).

(2) In the *compact description* one lists each $\mathbf{k}$ vector exactly once such that each point of the asymmetric unit is either an inner point itself or has inner points as neighbours. Such a description may not be uni-arm for some Wintgen positions, and the determination of the parameter ranges may become less straightforward.

(3) In the *non-unique description* one gives up the condition that each $\mathbf{k}$ vector is listed exactly once. The uni-arm and the compact descriptions are combined but the equivalence relations ($\sim$) are stated explicitly for those $\mathbf{k}$ vectors which occur in more than one entry. Such tables are most informative and not too complicated for practical applications.

### 1.5.6. Conclusions

*International Tables for Crystallography* Volume A can serve as a basis for the classification of irreps of space groups by using the concept of reciprocal-space groups. The main features of the crystallographic classification scheme are as follows.

(i) The asymmetric units of the conventional crystallographic unit cells are minimal domains of $\mathbf{k}$ space which are in many cases simpler than the representation domains of the Brillouin zones.

(ii) All $\mathbf{k}$-vector stars giving rise to the same type of irreps belong to the same Wintgen position and *vice versa*. They can be collected in one entry (uni-arm description) and are designated by the same Wintgen letter if flagpoles and wings are admitted.

(iii) The Wyckoff positions of *IT* A, interpreted as Wintgen positions, provide a complete list of the special $\mathbf{k}$ vectors in the Brillouin zone; the site symmetry of *IT* A is the little co-group $\overline{\mathcal{G}}^{\mathbf{k}}$ of $\mathbf{k}$; the multiplicity per primitive unit cell is the number of arms of the star of $\mathbf{k}$. The Wintgen positions with 0, 1, 2, or 3 variable parameters correspond to special $\mathbf{k}$-vector points, $\mathbf{k}$-vector lines, $\mathbf{k}$-vector planes or to the set of all general $\mathbf{k}$ vectors, respectively.

The complete set of types of irreps is obtained by considering the irreps of one $\mathbf{k}$ vector per Wintgen position in the uni-arm description. A complete set of inequivalent irreps of $\mathcal{G}$ is obtained from these irreps by varying the parameters within their ranges.

The authors wish to thank the editor of this volume, Uri Shmueli, for his patient support, for his encouragement and for his valuable help. They are grateful to the former Chairman of the Commission on *International Tables*, Theo Hahn, for his interest and advice. Part of the material in this chapter was first published as an article of the same title in *Z. Kristallogr.* (1995),



references