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 Γ, 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 $x, \frac{1}{2} - x, 0$, Σ 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.

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.

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 Φ 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 Λ 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 Ω in relation to the representation domain Φ is unnecessary. It may even be misleading because special $\mathbf{k}$-vector subspaces of Ω frequently belong to more general types of $\mathbf{k}$ vectors in Φ. 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.

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