International Tables for Crystallography (2010). Vol. B, Section 1.5.5.4.1, pp. 189–190.

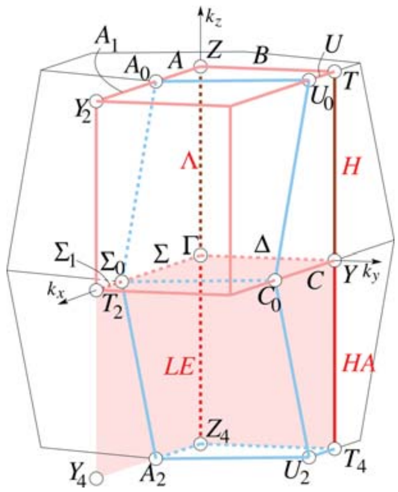

Fig. 1.5.5.7. Brillouin zone with asymmetric unit and representation domain of CDML for arithmetic crystal class $mm2F$: $a^{-2} > b^{-2} + c^{-2}$. Space groups $Fmm2 - C_{2v}^{18}$ (42), $Fdd2 - C_{2v}^{19}$ (43). Reciprocal-space group $(Imm2)$*, No. 44: $a^{*2} > b^{*2} + c^{*2}$ (see Table 1.5.5.7). The representation domain of CDML is different from the asymmetric unit. Auxiliary points: T_4: $0, \frac{1}{2}, -\frac{1}{2}$; Y_4: $\frac{1}{2}, 0, -\frac{1}{2}$; Z_4: $0, 0, -\frac{1}{2}$. Flagpoles: $LE = [Z_4\,\Gamma]$ $0, 0, z$: $-\frac{1}{2} < z < 0$; $HA = [T_4\,Y]$ $0, \frac{1}{2}, z$: $-\frac{1}{2} < z < 0$. Wings: $JA \cup J_3 = [\Gamma\, T_2\, Y_4\, Z_4]$ $x, 0, z$: $0 < x < \frac{1}{2}, -\frac{1}{2} < z < 0$; $EA = [\Gamma\, Z_4\, T_4\, Y]$ $0, y, z$: $0 < y < \frac{1}{2}, -\frac{1}{2} < z < 0$.

Brillouin zones are displayed in Fig. 1.5.5.5 (see also Table 1.5.5.5), Fig. 1.5.5.6 (see also Table 1.5.5.6) and Fig. 1.5.5.7 (see also Table 1.5.5.7). Fig. 1.5.5.5 is a distorted cuboctahedron with 14 faces, 36 edges and 24 apices, 18 of which are visible. The Brillouin zones of Figs. 1.5.5.6 and 1.5.5.7 are distorted elongated rhombdodecahedra. There are 12 faces, 28 edges and 18 apices; 14 of them are visible.

1.5.5.4. *Discussion*

1.5.5.4.1. *Representation domains and asymmetric units*

When the symmetry of the reciprocal lattice allows, the shape of the asymmetric unit may be chosen to be much simpler than that of the representation domain.

Examples

(1) Arithmetic crystal class $4/mmmI$. The parameter ranges for the special lines and planes of the asymmetric unit and for general **k** vectors of the reciprocal-space group $(F4/mmm)^*$ [setting $(I4/mmm)^*$] are listed in Tables 1.5.5.3 and 1.5.5.4. One can describe the corresponding conditions of the representation domain by the boundary plane $x, y, z = \{1 + (c/a)^2[1 - 2(x + y)]\}/4$ which for $c/a < 1$ forms the triangle $[Z_0\, Z_2\, P]$ in Fig. 1.5.5.3 but for $c/a > 1$ the pentagon $[S_2\, R\, P\, G\, S]$ in Fig. 1.5.5.4. The inner points of this boundary plane are points of the general position GP with the exception of the line $Q = x, \frac{1}{2} - x, \frac{1}{4}$, which is a twofold rotation axis. The boundary conditions for the representation domain depend on c/a; they are much more complicated than those, $x, y, z = \frac{1}{4}$, for the asymmetric unit.

(2) Arithmetic crystal class $mm2F$, see Figs. 1.5.5.5 to 1.5.5.7. In the reciprocal-space group $(Imm2)^*$ the lines Λ and LE belong to Wintgen position 2 a $mm2$, as do the lines Q, QA, Λ_1 and Λ_3 if present. The lines H and HA belong to the Wintgen position 2 b $mm2$; as do the lines G, GA, H_1 and H_3 if present. The lines Σ, Σ_1, A, A_1, C and U belong to the plane $x, 0, z$; the lines Δ, B, B_1 and D belong to the plane $0, y, z$. The decisive boundary plane of the representation domain is $xa^{*2} + yb^{*2} + zc^{*2} = d^{*2}/4$, where $d^{*2} = a^{*2} + b^{*2} + c^{*2}$; it is a hexagon for Fig. 1.5.5.5 and a parallelogram for Figs. 1.5.5.6 and 1.5.5.7. There is no relation of the lattice parameters for which all the above-mentioned lines are realized on the surface of the representation domain simultaneously; either two or

Table 1.5.5.7. *List of* **k**-*vector types for arithmetic crystal class mm2F*: $a^{-2} > b^{-2} + c^{-2}$

See Fig. 1.5.5.7. Parameter relations: $x = -\frac{1}{2}\alpha + \frac{1}{2}\beta + \frac{1}{2}\gamma$, $y = \frac{1}{2}\alpha - \frac{1}{2}\beta + \frac{1}{2}\gamma$, $z = \frac{1}{2}\alpha + \frac{1}{2}\beta - \frac{1}{2}\gamma$.

k-vector label, CDML	Wyckoff position of *IT* A, *cf.* Section 1.5.4.3	Parameters
Γ $0, 0, 0$	*ex* 2 *a* *mm*2	$0, 0, 0$
Z $\frac{1}{2}, \frac{1}{2}, 0$	*ex* 2 *a* *mm*2	$0, 0, \frac{1}{2}$
Λ $\alpha, \alpha, 0$	*ex* 2 *a* *mm*2	$0, 0, z$: $0 < z < \frac{1}{2}$
LE $-\alpha, -\alpha, 0$	*ex* 2 *a* *mm*2	$0, 0, z$: $-\frac{1}{2} < z < 0$
$\Gamma \cup Z \cup \Lambda \cup LE$	2 *a* *mm*2	$0, 0, z$: $-\frac{1}{2} < z \le \frac{1}{2}$
T $1, \frac{1}{2}, \frac{1}{2}$	*ex* 2 *b* *mm*2	$0, \frac{1}{2}, \frac{1}{2}$
Y $\frac{1}{2}, 0, \frac{1}{2}$	*ex* 2 *b* *mm*2	$0, \frac{1}{2}, 0$
H $\frac{1}{2} + \alpha, \alpha, \frac{1}{2}$	*ex* 2 *b* *mm*2	$0, \frac{1}{2}, z$: $0 < z < \frac{1}{2}$
HA $\frac{1}{2} - \alpha, -\alpha, \frac{1}{2}$	*ex* 2 *b* *mm*2	$0, \frac{1}{2}, z$: $-\frac{1}{2} < z < 0$
$T \cup Y \cup H \cup HA$	2 *b* *mm*2	$0, \frac{1}{2}, z$: $-\frac{1}{2} < z \le \frac{1}{2}$
Σ $0, \alpha, \alpha$	*ex* 4 *c* *.m.*	$x, 0, 0$: $0 < x \le \sigma_0$
U $1, \frac{1}{2} + \alpha, \frac{1}{2} + \alpha$	*ex* 4 *c* *.m.*	$x, \frac{1}{2}, \frac{1}{2}$: $0 < x < u_0$
$U \sim \Sigma_1 = [\Sigma_0\, T_2]$		$x, 0, 0$: $\frac{1}{2} - u_0 = \sigma_0 < x < \frac{1}{2}$
A $\frac{1}{2}, \frac{1}{2} + \alpha, \alpha$	*ex* 4 *c* *.m.*	$x, 0, \frac{1}{2}$: $0 < x < a_0$
C $\frac{1}{2}, \alpha, \frac{1}{2} + \alpha$	*ex* 4 *c* *.m.*	$x, \frac{1}{2}, 0$: $0 < x \le c_0$
$C \sim A_1 = [A_0\, Y_2]$		$x, 0, \frac{1}{2}$: $a_0 = \frac{1}{2} - c_0 \le x < \frac{1}{2}$
J $\alpha, \alpha + \beta, \beta$	*ex* 4 *c* *.m.*	$x, 0, z$: $[\Gamma\, Z\, A_0\, \Sigma_0]$
JA $-\alpha, -\alpha + \beta, \beta$	*ex* 4 *c* *.m.*	$x, 0, z$: $[\Gamma\, \Sigma_0\, A_2\, Z_4]$
K $\frac{1}{2} + \alpha, \alpha + \beta, \frac{1}{2} + \beta$	*ex* 4 *c* *.m.*	$x, \frac{1}{2}, z$: $[Y\, T\, U_0\, C_0]$
$K \sim J_3$		$x, 0, z$: $[T_2\, \Sigma_0\, A_2\, Y_4]$
KA $\frac{1}{2} - \alpha, -\alpha + \beta, \frac{1}{2} + \beta$	*ex* 4 *c* *.m.*	$x, \frac{1}{2}, z$: $[Y\, C_0\, U_2\, T_4]$
$KA \sim J_1$		$x, 0, z$: $[T_2\, \Sigma_0\, A_0\, Y_2]$
$A \cup A_1 \cup J \cup J_1 \cup \Sigma \cup \Sigma_1 \cup JA \cup J_3$	4 *c* *.m.*	$x, 0, z$: $0 < x < \frac{1}{2}, -\frac{1}{2} < z \le \frac{1}{2}$
Δ $\alpha, 0, \alpha$	*ex* 4 *d* *m..*	$0, y, 0$: $0 < y < \frac{1}{2}$
B $\frac{1}{2} + \alpha, \frac{1}{2}, \alpha$	*ex* 4 *d* *m..*	$0, y, \frac{1}{2}$: $0 < y < \frac{1}{2}$
E $\alpha + \beta, \alpha, \beta$	*ex* 4 *d* *m..*	$0, y, z$: $0 < y, z < \frac{1}{2}$
EA $-\alpha + \beta, -\alpha, \beta$	*ex* 4 *d* *m..*	$0, y, z$: $0 < y < \frac{1}{2}, -\frac{1}{2} < z < 0$
$\Delta \cup B \cup E \cup EA$	4 *d* *m..*	$0, y, z$: $0 < y < \frac{1}{2}, -\frac{1}{2} < z \le \frac{1}{2}$
GP α, β, γ	8 *e* 1	x, y, z: $0 < x, y < \frac{1}{2}, 0 \le z < \frac{1}{2}$

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 Λ (α, α, α) 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 Λ connects the points Γ 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 analoguous 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 Λ 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 (Γ, H, N) and lines (Δ, Σ, G) of the boundary of the asymmetric unit are special. In $(Fm\overline{3})^*$, see Fig. 1.5.5.2, the lines Δ and $[\Gamma\, H_2] \sim \Delta$ are special but Σ, 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; $\bar{x}, x, z$; x, y, x; $x, y, \bar{x}$; x, y, y; $x, \bar{y}, y$. Three of them (x, x, z, $\bar{x}, x, z$ 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) $m..$,

references