International Tables for Crystallography (2010). Vol. B, Section 1.5.5.3, pp. 188–189.

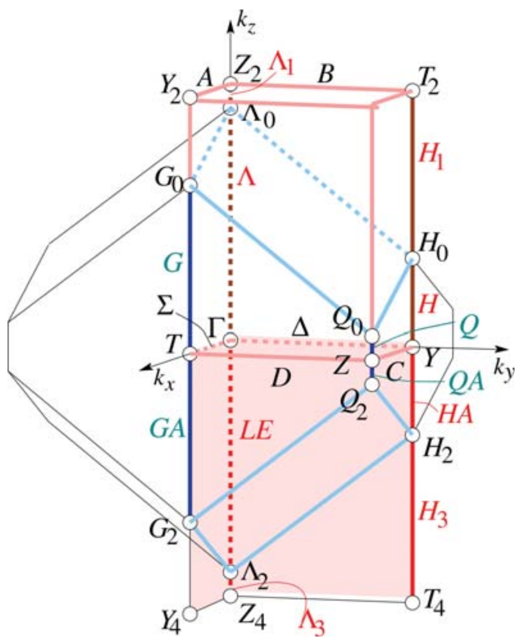

Fig. 1.5.5.6. Brillouin zone with asymmetric unit and representation domain of CDML for arithmetic crystal class $mm2F$: $c^{-2} > a^{-2} + b^{-2}$. Space groups $Fmm2 - C_{2v}^{18}$ (42), $Fdd2 - C_{2v}^{19}$ (43). Reciprocal-space group $(Imm2)$*, No. 44: $c^{*2} > a^{*2} + b^{*2}$ (see Table 1.5.5.6). 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: $0, 0, z$: $-\frac{1}{2} < z < 0$; $0, \frac{1}{2}, z$: $-\frac{1}{2} < z < 0$. Wings: $x, 0, z$: $0 < x < \frac{1}{2}, -\frac{1}{2} < z < 0$; $0, y, z$: $0 < y < \frac{1}{2}$, $-\frac{1}{2} < z < 0$.

Table 1.5.5.6. *List of* **k***-vector types for arithmetic crystal class mm2F:* $c^{-2} > a^{-2} + b^{-2}$

See Fig. 1.5.5.6. 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 $\frac{1}{2}, \frac{1}{2}, 1$	*ex* 2 *a* *mm*2	$\frac{1}{2}, \frac{1}{2}, 0$
$Z \sim Z_2$		$0, 0, \frac{1}{2}$
Λ $\alpha, \alpha, 0$	*ex* 2 *a* *mm*2	$0, 0, z$: $0 < z \le \lambda_0$
LE $-\alpha, -\alpha, 0$	*ex* 2 *a* *mm*2	$0, 0, z$: $\lambda_2 = -\lambda_0 < z < 0$
Q $\frac{1}{2} + \alpha, \frac{1}{2} + \alpha, 1$	*ex* 2 *a* *mm*2	$\frac{1}{2}, \frac{1}{2}, z$: $0 < z \le q_0$
$Q \sim \Lambda_3 = [\Lambda_2 Z_4]$		$0, 0, z$: $-\frac{1}{2} < z \le -\frac{1}{2} + q_0 = -\lambda_0$
QA $\frac{1}{2} - \alpha, \frac{1}{2} - \alpha, 1$	*ex* 2 *a* *mm*2	$\frac{1}{2}, \frac{1}{2}, z$: $q_2 = -q_0 < z < 0$
$QA \sim \Lambda_1 = [\Lambda_0 Z_2]$		$0, 0, z$: $\frac{1}{2} - q_0 = \lambda_0 < z < \frac{1}{2}$
$Z_2 \cup \Lambda_1 \cup \Lambda \cup \Gamma \cup LE \cup \Lambda_3$	2 *a* *mm*2	$0, 0, z$: $-\frac{1}{2} < z \le \frac{1}{2}$
T $0, \frac{1}{2}, \frac{1}{2}$	*ex* 2 *b* *mm*2	$\frac{1}{2}, 0, 0$
$T \sim T_2$		$0, \frac{1}{2}, \frac{1}{2}$
Y $\frac{1}{2}, 0, \frac{1}{2}$	*ex* 2 *b* *mm*2	$0, \frac{1}{2}, 0$
G $\alpha, \frac{1}{2} + \alpha, \frac{1}{2}$	*ex* 2 *b* *mm*2	$\frac{1}{2}, 0, z$: $0 < z \le g_0$
$G \sim H_3 = [H_2 T_4]$		$0, \frac{1}{2}, z$: $-\frac{1}{2} < z \le -\frac{1}{2} + g_0$
GA $-\alpha, \frac{1}{2} - \alpha, \frac{1}{2}$	*ex* 2 *b* *mm*2	$\frac{1}{2}, 0, z$: $g_2 = -g_0 < z < 0$
$GA \sim H_1 = [H_0 T_2]$		$0, \frac{1}{2}, z$: $\frac{1}{2} - g_0 = h_0 < z < \frac{1}{2}$
H $\frac{1}{2} + \alpha, \alpha, \frac{1}{2}$	*ex* 2 *b* *mm*2	$0, \frac{1}{2}, z$: $0 < z \le h_0$
HA $\frac{1}{2} - \alpha, -\alpha, \frac{1}{2}$	*ex* 2 *b* *mm*2	$0, \frac{1}{2}, z$: $h_2 = -h_0 < z < 0$
$T_2 \cup H_1 \cup H \cup Y \cup HA \cup H_3$	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.*	$x, 0, 0$: $0 < x < \frac{1}{2}$
C $\frac{1}{2}, \alpha, \frac{1}{2} + \alpha$	*ex* 4 *c* *.m.*	$x, \frac{1}{2}, 0$: $0 < x < \frac{1}{2}$
$C \sim A = [Z_2 Y_2]$		$x, 0, \frac{1}{2}$: $0 < z < \frac{1}{2}$
J $\alpha, \alpha + \beta, \beta$	*ex* 4 *c* *.m.*	$x, 0, z$: $[\Gamma \Lambda_0 G_0 T]$
JA $-\alpha, -\alpha + \beta, \beta$	*ex* 4 *c* *.m.*	$x, 0, z$: $[\Gamma T G_2 \Lambda_2]$
K $\frac{1}{2} + \alpha, \alpha + \beta, \frac{1}{2} + \beta$	*ex* 4 *c* *.m.*	$x, \frac{1}{2}, z$: $[Y H_0 Q_0 Z]$
$K \sim J_3$		$x, 0, z$: $[Y_4 G_2 \Lambda_2 Z_4]$
KA $\frac{1}{2} - \alpha, -\alpha + \beta, \frac{1}{2} + \beta$	*ex* 4 *c* *.m.*	$x, \frac{1}{2}, z$: $[Z Q_2 H_2 Y]$
$KA \sim J_1$		$x, 0, z$: $[Z_2 Y_2 G_0 \Lambda_0]$
$A \cup J_1 \cup J \cup \Sigma \cup JA \cup J_3$	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..*	$0, y, 0$: $0 < y < \frac{1}{2}$
D $\alpha, \frac{1}{2}, \frac{1}{2} + \alpha$	*ex* 4 *d* *m..*	$\frac{1}{2}, y, 0$: $0 < y < \frac{1}{2}$
$D \sim B$		$0, y, \frac{1}{2}$: $0 < y < \frac{1}{2}$
E $\alpha + \beta, \alpha, \beta$	*ex* 4 *d* *m..*	$0, y, z$: $[\Gamma Y H_0 \Lambda_0]$
EA $-\alpha + \beta, -\alpha, \beta$	*ex* 4 *d* *m..*	$0, y, z$: $[\Gamma \Lambda_2 H_2 Y]$
F $\alpha + \beta, \frac{1}{2} + \alpha, \frac{1}{2} + \beta$	*ex* 4 *d* *m..*	$\frac{1}{2}, y, z$: $[T Z Q_0 G_0]$
$F \sim E_3$		$0, y, z$: $[Z_4 \Lambda_2 H_2 T_4]$
FA $-\alpha + \beta, \frac{1}{2} - \alpha, \frac{1}{2} + \beta$	*ex* 4 *d* *m..*	$\frac{1}{2}, y, z$: $[T G_2 Q_2 Z]$
$FA \sim E_1$		$0, y, z$: $[Z_2 \Lambda_0 H_0 T_2]$
$B \cup E_1 \cup E \cup \Delta \cup EA \cup E_3$	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: $0 < x, y < \frac{1}{2}$; $0 < z \le \frac{1}{2}$

In general the sequence of the Wyckoff letters in *IT* A follows the falling number of free parameters. In the few cases where the sequence in *IT* A is different, the Wyckoff letters are exchanged. The exchange is noted at the top of the table.

Example. In the arithmetic crystal class $4/mmmI$, $c/a < 1$, see Table 1.5.5.3, Wyckoff position *e* has one free parameter, whereas Wyckoff position *f* has constant parameters, *i.e.* no free parameter. Therefore, *f* is listed above the horizontal line, *e* is listed below, see Table 1.5.5.3. The note at the top of the table states 'Wyckoff positions *e* and *f* exchanged'.

Parameter relations. The relations between the parameters of CDML and the parameters referred to the asymmetric unit are listed at the top of the table, *e.g.* for $m\bar{3}mI$ in Table 1.5.5.1: 'Parameter relations: $x = \frac{1}{2}\beta + \frac{1}{2}\gamma$, $y = \frac{1}{2}\alpha + \frac{1}{2}\gamma$, $z = \frac{1}{2}\alpha + \frac{1}{2}\beta$'. These relations may be modified to more convenient parameters without notice, as for the plane B of $m\bar{3}mI$ in Table 1.5.5.1:

$$B \quad \alpha + \beta, -\alpha + \beta, \tfrac{1}{2} - \beta \quad ex\ 96\ k\ ..m \quad x, \tfrac{1}{2} - x, z\text{: } 0 < z < x < \tfrac{1}{4}$$

instead of

$$\ldots \tfrac{1}{4} - \tfrac{1}{2}\alpha, \tfrac{1}{4} + \tfrac{1}{2}\alpha, \beta\text{: } 0 < \alpha < \tfrac{1}{2} - 2\beta < \tfrac{1}{2}.$$

1.5.5.3. Figures and tables

Arithmetic crystal classes $m\bar{3}mI$ *and* $m\bar{3}I$: The reciprocal lattice of a cubic lattice *I* is a cubic lattice *F*. Its Brillouin zone is a rhombic dodecahedron and has 12 faces, 24 edges and 14 apices, the coordinates of which are the six permutations of $\pm\frac{1}{2}, 0, 0$ and the eight coordinate triplets of $\pm\frac{1}{4}, \pm\frac{1}{4}, \pm\frac{1}{4}$. Eleven of these 14 points are visible in the applied projection.

The figure for arithmetic crystal class $m\bar{3}mI$ is shown in Fig. 1.5.5.1 and the corresponding table is Table 1.5.5.1. The figure for arithmetic crystal class $m\bar{3}I$ is shown in Fig. 1.5.5.2 and the corresponding table is Table 1.5.5.2.

Arithmetic crystal class $4/mmmI$: There are two different types of Brillouin zones for the tetragonal *I* lattice, one for $c < a$ (Fig. 1.5.5.3, Table 1.5.5.3) and one for $c > a$ (Fig. 1.5.5.4, Table 1.5.5.4). The first type of Brillouin zone, Fig. 1.5.5.3, is a tetragonal elongated rhombdodecahedron with 12 faces, four of them being hexagons. There are 18 apices; 14 of them are visible. The Brillouin zone of Fig. 1.5.5.4 is a tetragonally deformed cuboctahedron with 14 faces. There are 24 apices; 18 of them are visible.

Arithmetic crystal class mm2F: Depending on the lattice ratios *a*:*b*:*c*, there are four figures in CDML for the Brillouin zone of an orthorhombic crystal with an *F* lattice, see Fig. 3.6 on p. 26 in CDML. Only three of them are really necessary. Therefore, the case $b^{-2} > c^{-2} + a^{-2}$ of Fig. 3.6(c) of CDML has been omitted in these examples; it is obtained from $a^{-2} > c^{-2} + b^{-2}$ of Figure 3.6(d) by a rotation by 90° about the c^* axis. The three remaining

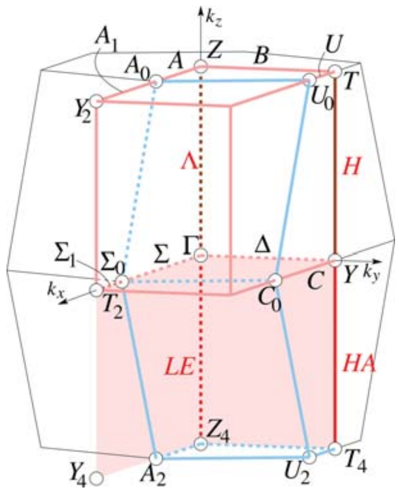

Fig. 1.5.5.7. Brillouin zone with asymmetric unit and representation domain of CDML for arithmetic crystal class $mm2F$: $a^{-2} > b^{-2} + c^{-2}$. Space groups $Fmm2 - C_{2v}^{18}$ (42), $Fdd2 - C_{2v}^{19}$ (43). Reciprocal-space group $(Imm2)^*$, No. 44: $a^{*2} > b^{*2} + c^{*2}$ (see Table 1.5.5.7). 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* $mm2$	$0, 0, 0$
Z $\frac{1}{2}, \frac{1}{2}, 0$	*ex* 2 *a* $mm2$	$0, 0, \frac{1}{2}$
Λ $\alpha, \alpha, 0$	*ex* 2 *a* $mm2$	$0, 0, z$: $0 < z < \frac{1}{2}$
LE $-\alpha, -\alpha, 0$	*ex* 2 *a* $mm2$	$0, 0, z$: $-\frac{1}{2} < z < 0$
$\Gamma \cup Z \cup \Lambda \cup LE$	2 *a* $mm2$	$0, 0, z$: $-\frac{1}{2} < z \le \frac{1}{2}$
T $1, \frac{1}{2}, \frac{1}{2}$	*ex* 2 *b* $mm2$	$0, \frac{1}{2}, \frac{1}{2}$
Y $\frac{1}{2}, 0, \frac{1}{2}$	*ex* 2 *b* $mm2$	$0, \frac{1}{2}, 0$
H $\frac{1}{2} + \alpha, \alpha, \frac{1}{2}$	*ex* 2 *b* $mm2$	$0, \frac{1}{2}, z$: $0 < z < \frac{1}{2}$
HA $\frac{1}{2} - \alpha, -\alpha, \frac{1}{2}$	*ex* 2 *b* $mm2$	$0, \frac{1}{2}, z$: $-\frac{1}{2} < z < 0$
$T \cup Y \cup H \cup HA$	2 *b* $mm2$	$0, \frac{1}{2}, z$: $-\frac{1}{2} < z \le \frac{1}{2}$
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: $0 < x, y < \frac{1}{2}, 0 \le z < \frac{1}{2}$

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