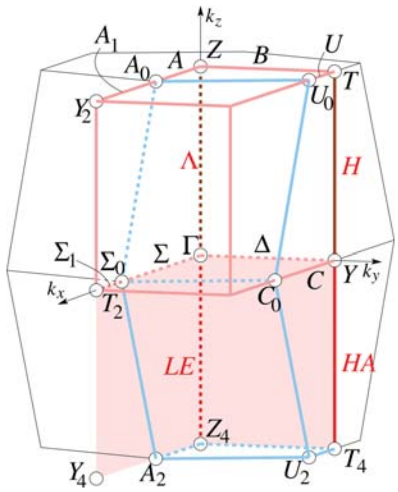

Fig. 1.5.5.7. Brillouin zone with asymmetric unit and representation domain of CDML for arithmetic crystal class $mm2F$: $a^{-2} > b^{-2} + c^{-2}$. Space groups $Fmm2 - C_{2v}^{18}$ (42), $Fdd2 - C_{2v}^{19}$ (43). Reciprocal-space group $(Imm2)^*$, No. 44: $a^{*2} > b^{*2} + c^{*2}$ (see Table 1.5.5.7).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