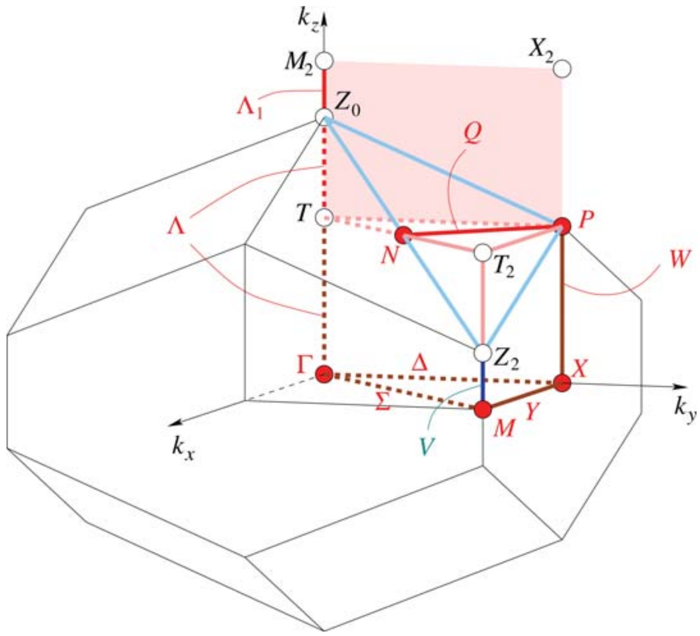

Fig. 1.5.5.3. Brillouin zone with asymmetric unit and representation domain of CDML for arithmetic crystal class $4/mmmI$: $c/a < 1$. Space groups $I4/mmm - D_{4h}^{17}$ (139) to $I4_1/acd - D_{4h}^{20}$ (142). Reciprocal-space group $(I4/mmm)^*$, No. 139: $c^*/a^* > 1$ (see Table 1.5.5.3). The representation domain of CDML is different from the asymmetric unit. Auxiliary points: T: $0, 0, \frac{1}{4}$; T_2: $\frac{1}{2}, \frac{1}{2}, \frac{1}{4}$; X_2: $0, \frac{1}{2}, \frac{1}{2}$. Flagpole: $[T\,M_2]$ $0, 0, z$: $\frac{1}{4} < z < \frac{1}{2}$. Wing: $[T\,P\,X_2\,M_2]$ $0, y, z$: $0 < y < \frac{1}{2}, \frac{1}{4} < z < \frac{1}{2}$.

vector, multiplied by the number of centring vectors of the conventional unit cell in *IT* A.

Unlike in *IT* A, each table starts with the Wyckoff letter *a* for a Wyckoff position of highest site symmetry and proceeds in alphabetical order until the general position *GP* is reached. The sequence of the CDML labels is not that of CDML but is determined essentially by the alphabetical sequence of the Wyckoff positions.

The symbol for the site symmetry is 'oriented', as given in the space-group tables of *IT* A. For the nomenclature, see Section 2.2.12 of *IT* A.

Column 3. These are the parameters of that Wyckoff position of $\mathcal{G}_0$ which corresponds to the **k**-vector label in CDML, see Column 1. The *parameter description* and the *parameter range* are listed. This range is chosen such that each orbit of the Wyckoff position of *IT* A, *i.e.* also each **k**-vector orbit, is listed exactly once.

The following designation is used for the parameter ranges:

(1) The statement $0 < x,\ y < \frac{1}{2}$ means that x and y may vary independently from 0 to $\frac{1}{2}$, 0 and $\frac{1}{2}$ both excluded.

(2) The statement

$$GP \quad \alpha, \beta, \gamma \quad 48\ h\ 1 \quad x, y, z: 0 \le z < x < y < \tfrac{1}{2} \cup \cup\, x, \tfrac{1}{2}, z: 0 < z < x < \tfrac{1}{2}$$

means that the description of the asymmetric unit is split into two adjacent regions, a body and a plane. The boundary plane $z = 0$ of the body is included, all other boundaries are excluded. Together the regions contain exactly one representative for each **k**-vector orbit of the general position *GP* of the reciprocal-space group.

(3) The statement $x, \frac{1}{2}, z$: $-x < z \le x,\ z \ne 0$ means that z may assume any value between $-x$ and $+x$, $z = x$ included but $z = -x$ and $z = 0$ excluded.

(4) Occasionally the parameter description becomes too clumsy. Then the data listed are abbreviated by replacing the parametrical data by the designation of the corresponding region.

Table 1.5.5.3. *List of* **k***-vector types for arithmetic crystal class* $4/mmmI$*:* $c/a < 1$

See Fig. 1.5.5.3. Wyckoff positions *e* and *f* exchanged. Parameter relations: $x = -\frac{1}{2}\alpha + \frac{1}{2}\beta$, $y = \frac{1}{2}\alpha + \frac{1}{2}\beta + \gamma$, $z = \frac{1}{2}\alpha + \frac{1}{2}\beta$.

k-vector label, CDML	Wyckoff position of *IT* A, *cf.* Section 1.5.4.3	Parameters
Γ $0, 0, 0$	2 *a* $4/mmm$	$0, 0, 0$
M $-\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	2 *b* $4/mmm$	$\frac{1}{2}, \frac{1}{2}, 0$
$M \sim M_2$		$0, 0, \frac{1}{2}$
X $0, 0, \frac{1}{2}$	4 *c* $mmm.$	$0, \frac{1}{2}, 0$
P $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	4 *d* $\bar{4}m2$	$0, \frac{1}{2}, \frac{1}{4}$
N $0, \frac{1}{2}, 0$	8 *f* $..2/m$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$
Λ $\alpha, \alpha, -\alpha$	*ex* 4 *e* $4mm$	$0, 0, z$: $0 < z \le z_0$
V $-\frac{1}{2}+\alpha, \frac{1}{2}+\alpha, \frac{1}{2}-\alpha$	*ex* 4 *e* $4mm$	$\frac{1}{2}, \frac{1}{2}, z$: $0 < z < z_2 = \frac{1}{2} - z_0$
$V \sim \Lambda_1 = [Z_0\,M_2]$		$0, 0, z$: $z_0 < z < \frac{1}{2}$
$\Lambda \cup \Lambda_1 = [\Gamma\,M_2]$	4 *e* $4mm$	$0, 0, z$: $0 < z < \frac{1}{2}$
W $\alpha, \alpha, \frac{1}{2}-\alpha$	8 *g* $2mm.$	$0, \frac{1}{2}, z$: $0 < z < \frac{1}{4}$
Σ $-\alpha, \alpha, \alpha$	8 *h* $m.2m$	$x, x, 0$: $0 < x < \frac{1}{2}$
Δ $0, 0, \alpha$	8 *i* $m2m.$	$0, y, 0$: $0 < y < \frac{1}{2}$
Y $-\alpha, \alpha, \frac{1}{2}$	8 *j* $m2m.$	$x, \frac{1}{2}, 0$: $0 < x < \frac{1}{2}$
Q $\frac{1}{4}-\alpha, \frac{1}{4}+\alpha, \frac{1}{4}-\alpha$	16 *k* $..2$	$x, \frac{1}{2}-x, \frac{1}{4}$: $0 < x < \frac{1}{4}$
C $-\alpha, \alpha, \beta$	16 *l* $m..$	$x, y, 0$: $0 < x < y < \frac{1}{2}$
B $\alpha, \beta, -\alpha$	16 *m* $..m$	x, x, z: $[\Gamma\,M\,Z_2\,Z_0]$
$B = B_1 \cup B_2$ $= [\Gamma\,M\,Z_2\,N\,T] \cup [T\,N\,Z_0]$		
$B_2 \sim B_3$		x, x, z: $[N\,Z_2\,T_2]$
$B_1 \cup B_3 = [\Gamma\,M\,T_2\,T]$	16 *m* $..m$	x, x, z: $0 < x < \frac{1}{2}$, $0 < z < \frac{1}{4}$ $\cup$ $\cup\ x, x, \frac{1}{4}$: $0 < x < \frac{1}{4}$
A α, α, β	*ex* 16 *n* $.m.$	$0, y, z$: $[\Gamma\,X\,P\,Z_0]$
E $\alpha-\beta, \alpha+\beta, \frac{1}{2}-\alpha$	*ex* 16 *n* $.m.$	$x, \frac{1}{2}, z$: $[M\,X\,P\,Z_2]$
$E \sim A_1$		$0, y, z$: $[P\,X_2\,M_2\,Z_0]$
$A \cup A_1 = [\Gamma\,X\,X_2\,M_2]$	16 *n* $.m.$	$0, y, z$: $0 < y, z < \frac{1}{2}$
GP α, β, γ	32 *o* 1	x, y, z: $0 < x < y < \frac{1}{2}$; $0 < z < \frac{1}{4}$ $\cup$ $\cup\ x, y, \frac{1}{4}$: $0 < x < y < \frac{1}{2} - x$

references