*International Tables for Crystallography* (2010). Vol. B, Section 1.5.5.2, pp. 184–188.



metric unit may be selected as orbit representatives. Such a piece of a plane is called a *wing*. Wings are always coloured pink, see, *e.g.*, Fig. 1.5.5.1.

Within the caption of each figure the following data are listed:

(i) a statement of whether the representation domain and the asymmetric unit are identical or not;

(ii) the coordinates of auxiliary points if not specified in the corresponding table;

(iii) the parameter descriptions of the flagpoles and the wings.

### 1.5.5.2. *Guide to the* **k***-vector tables*

Each figure is followed by a table with the same number. As for the figures, each table caption gives the name of the arithmetic crystal class of space groups. If there is more than one table for this arithmetic crystal class, then the symbol for the arithmetic crystal class is followed by the specific conditions for the lattice parameters, as for the figures.

*Column 1*. Label of the **k** vectors in CDML, Tables 3.9 and 3.11 and parameter description of CDML for the set of **k** vectors which belong to the label. No ranges for the parameters are listed in CDML.

If two **k** vectors belong to the same type of **k** vectors, then their little co-groups are conjugate under the reciprocal-space group $(\mathcal{G})^*$ and they correspond to the same Wyckoff position. Different **k** vectors with the *same* CDML label always belong to the same **k**-vector type. **k** vectors with *different* CDML labels may either belong to the same or to different types of **k** vectors. If such **k** vectors belong to the same type, the corresponding Wyckoff-position descriptions are preceded by the letters '*ex*'. Frequently, such **k** vectors have been transformed (sign '$\sim$' in these tables) to equivalent ones in order to make the **k** vectors uni-arm, see the tables in this section.

The parameter range of a region may be described by the vertices of that region in brackets [...]. One point in brackets, *e.g.* [$P$], means the point $P$. Two points within the brackets, *e.g.* [$A\ B$] means the line from $A$ to $B$. Three points within the brackets, *e.g.* [$A\ B\ C$] means the triangular region of a plane with the vertices $A$, $B$ and $C$. Four or more points may mean a region of a plane or a three-dimensional body, depending on the positions of the points. The meaning can be recognized by studying the corresponding figure. Commas between the points, *e.g.* [$A, B, C$] indicate the set $\{A, B, C\}$ of the three points $A$, $B$ and $C$.

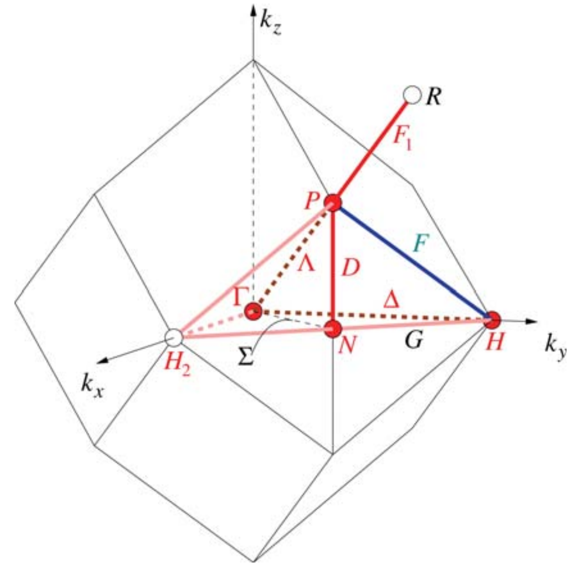


Fig. 1.5.5.2. Brillouin zone with asymmetric unit and representation domain of CDML for arithmetic crystal class $m\bar{3}I$. Space groups $Im\bar{3} - T_h^5$ (204), $Ia\bar{3} - T_h^7$ (206). Reciprocal-space group $(Fm\bar{3})^*$, No. 202 (see Table 1.5.5.2). The representation domain of CDML is identical with the asymmetric unit. Auxiliary points: $R$: $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$; $H_2$: $\frac{1}{2}, 0, 0$. Flagpole: $F_1 = [P\,R]$ $x, x, x$: $\frac{1}{4} < x < \frac{1}{2}$.

A symbol [...] does not indicate whether the vertices, boundary lines or boundary planes of the region are themselves included or not. All or part of them may belong to the region, all or part of them may not. In the parameter description of the region in Column 3 the inclusion or exclusion is stated by the symbols $\leq$ or $<$.

The backslash '\' is used to indicate included parts not belonging to the described region, see *e.g.* the regions $[\Gamma\,R]\backslash[P]$ and $[\Gamma\,N\,N_2\,H_2]\backslash[\Lambda,\ F_3]$ in Table 1.5.5.1.

*Column 2*. This column describes the Wyckoff positions (given as the multiplicity, the Wyckoff letter and the site symmetry) of that symmorphic space group $\mathcal{G}_0$ of *IT* A which is isomorphic to the reciprocal-space group $(\mathcal{G})^*$. Each Wyckoff position of $\mathcal{G}_0$ corresponds to a Wintgen position of $(\mathcal{G})^*$, *i.e.* to a type of **k** vectors of $(\mathcal{G})^*$ and *vice versa*.

'Multiplicity' is the number of points in the conventional unit cell of *IT* A. Here it is the number of arms of the star of the **k**

Table 1.5.5.2. *List of* **k***-vector types for arithmetic crystal class* $m\bar{3}I$

See Fig. 1.5.5.2. Parameter relations: $x = \frac{1}{2}\beta + \frac{1}{2}\gamma$, $y = \frac{1}{2}\alpha + \frac{1}{2}\gamma$, $z = \frac{1}{2}\alpha + \frac{1}{2}\beta$.

| **k**-vector label, CDML | Wyckoff position of *IT* A, *cf.* Section 1.5.4.3 | Parameters |
|---|---|---|
| $\Gamma$ 0, 0, 0 | 4 *a* $m\bar{3}.$ | 0, 0, 0 |
| $H$ $\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}$ | 4 *b* $m\bar{3}.$ | $0, \frac{1}{2}, 0$ |
| $P$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | 8 *c* 23. | $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ |
| $N$ $0, 0, \frac{1}{2}$ | 24 *d* $2/m..$ | $\frac{1}{4}, \frac{1}{4}, 0$ |
| $\Delta$ $\alpha, -\alpha, \alpha$ | 24 *e* $mm2..$ | $0, y, 0$: $0 < y < \frac{1}{2}$ |
| $\Lambda$ $\alpha, \alpha, \alpha$ | *ex* 32 *f* .3. | $x, x, x$: $0 < x < \frac{1}{4}$ |
| $F$ $\frac{1}{2}-\alpha, -\frac{1}{2}+3\alpha, \frac{1}{2}-\alpha$ | *ex* 32 *f* .3. | $x, \frac{1}{2}-x, x$: $0 < x < \frac{1}{4}$ |
| $F \sim F_1 = [P\,R]$ | | $x, x, x$: $\frac{1}{4} < x < \frac{1}{2}$ |
| $\Lambda \cup F_1 \sim [\Gamma\,R]\backslash[P]$ | 32 *f* .3. | $x, x, x$: $0 < x < \frac{1}{2}, x \neq \frac{1}{4}$ |
| $D$ $\alpha, \alpha, \frac{1}{2}-\alpha$ | 48 *g* 2.. | $\frac{1}{4}, \frac{1}{4}, z$: $0 < z < \frac{1}{4}$ |
| $\Sigma$ $0, 0, \alpha$ | *ex* 48 *h* *m..* | $x, x, 0$: $0 < x < \frac{1}{4}$ |
| $G$ $\frac{1}{2}-\alpha, -\frac{1}{2}+\alpha, \frac{1}{2}$ | *ex* 48 *h* *m..* | $x, \frac{1}{2}-x, 0$: $0 < x < \frac{1}{4}$ |
| $A = [\Gamma\,N\,H]$ $\alpha, -\alpha, \beta$ | *ex* 48 *h* *m..* | $x, y, 0$: $0 < x < y < \frac{1}{2}-x$ |
| $AA = [\Gamma\,H_2\,N]$ $-\alpha, \alpha, \beta$ | *ex* 48 *h* *m..* | $x, y, 0$: $0 < y < x < \frac{1}{2}-y$ |
| $\Sigma \cup G \cup A \cup AA$ | 48 *h* *m..* | $x, y, 0$: $0 < y < \frac{1}{2}-x < \frac{1}{2}$ $\cup$ $\cup\ x, \frac{1}{2}-x, 0$: $0 < x < \frac{1}{4}$ |
| $GP$ $\alpha, \beta, \gamma$ | 96 *i* 1 | $x, y, z$: $0 < z \leq x < y < \frac{1}{2}-x$ $\cup$ $\cup\ x, y, z$: $0 < z < y < x \leq \frac{1}{2}-y$ $\cup$ $\cup\ x, x, z$: $0 < z < x < \frac{1}{4}$ |

 

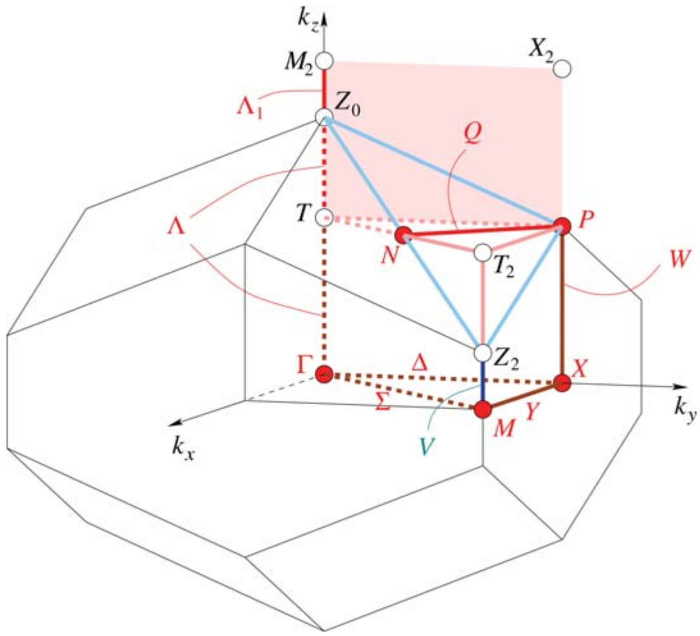


Fig. 1.5.5.3. Brillouin zone with asymmetric unit and representation domain of CDML for arithmetic crystal class $4/mmmI$: $c/a < 1$. Space groups $I4/mmm - D_{4h}^{17}$ (139) to $I4_1/acd - D_{4h}^{20}$ (142). Reciprocal-space group $(I4/mmm)$*, No. 139: $c^*/a^* > 1$ (see Table 1.5.5.3). The representation 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 |
|---|---|---|
| $\Gamma$ $0, 0, 0$ | 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* $..2/m$ | $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ |
| $\Lambda$ $\alpha, \alpha, -\alpha$ | *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* $2mm.$ | $0, \frac{1}{2}, z$: $0 < z < \frac{1}{4}$ |
| $\Sigma$ $-\alpha, \alpha, \alpha$ | 8 *h* $m.2m$ | $x, x, 0$: $0 < x < \frac{1}{2}$ |
| $\Delta$ $0, 0, \alpha$ | 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* $..m$ | $x, x, z$: $0 < x < \frac{1}{2}$, $0 < z < \frac{1}{4}$ $\cup$ $\cup$ $x, x, \frac{1}{4}$: $0 < x < \frac{1}{4}$ |
| $A$ $\alpha, \alpha, \beta$ | *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* $.m.$ | $0, y, z$: $0 < y, z < \frac{1}{2}$ |
| $GP$ $\alpha, \beta, \gamma$ | 32 *o* $1$ | $x, y, z$: $0 < x < y < \frac{1}{2}$; $0 < z < \frac{1}{4}$ $\cup$ $\cup$ $x, y, \frac{1}{4}$: $0 < x < y < \frac{1}{2} - x$ |

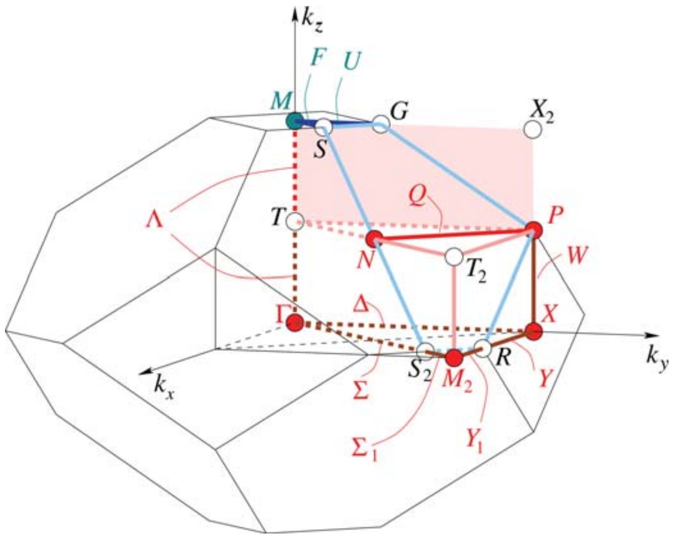


Fig. 1.5.5.4. Brillouin zone with asymmetric unit and representation domain of CDML for arithmetic crystal class $4/mmmI$: $c/a > 1$. Space groups $I4/mmm - D_{4h}^{17}$ (139) to $I4_1/acd - D_{4h}^{20}$ (142). Reciprocal-space group $(I4/mmm)$*, No. 139: $c^*/a^* < 1$ (see Table 1.5.5.4). The representation domain of CDML is different from the asymmetric unit. Auxiliary points: $X_2$: $0, \frac{1}{2}, \frac{1}{2}$; $T$: $0, 0, \frac{1}{4}$; $T_2$: $\frac{1}{2}, \frac{1}{2}, \frac{1}{4}$. Flagpole: $[T\,M]$ $0, 0, z$: $\frac{1}{4} < z < \frac{1}{2}$. Wing: $[T\,P\,X_2\,M]$ $0, y, z$: $0 < y < \frac{1}{2}, \frac{1}{4} < z < \frac{1}{2}$.

*Example*. In Table 1.5.5.3 one finds for the arithmetic crystal class $4/mmmI$ of space groups:

$$B \quad \alpha, \beta, -\alpha \quad 16\ m\ ..m \quad x, x, z\text{: } [\Gamma\, M\, Z_2\, Z_0]$$

The parameter description would be:

$$x, x, z\text{: } 0 < x < \tfrac{1}{2},\ 0 < z \le z_0 - 2x(2z_0 - \tfrac{1}{2})$$

*Horizontal lines*. The horizontal lines extending across the tables separate blocks with different numbers of free parameters. Decisive for this subdivision is the number of free parameters of the Wyckoff position to which the Wintgen position is assigned, not the number of free parameters of CDML.

*Example. Arithmetic crystal class mm2F, see Table 1.5.5.5*
The **k**-vector labels '$\Gamma$ $0, 0, 0$' and '$Z$ $\frac{1}{2}, \frac{1}{2}, 0$' of CDML have no free parameter. However, they correspond to the Wyckoff position '2 $a$ $mm2$ $0, 0, z$', which has one free parameter. Therefore, $\Gamma$ and $Z$ are listed together with '$\Lambda$ $\alpha, \alpha, 0$' and '$LE$ $-\alpha, -\alpha, 0$' in the block for the symmetry lines, *i.e.* for the **k** vectors with one free parameter: in $(Imm2)^*$ there is no parameter-free Wintgen position at all. The **k**-vector labels '$\Sigma$ $0, \alpha, \alpha$' and '$A$ $\frac{1}{2}, \frac{1}{2} + \alpha, \alpha$' of CDML have one free parameter each. However, they correspond together with other **k**-vector labels to the Wyckoff position '4 $c$ $.m.$ $x, 0, z$'. Therefore, $\Sigma$ and $A$ are listed together with '$J$ $\alpha, \alpha + \beta, \beta$' and '$JA$ $-\alpha, -\alpha + \beta, \beta$' and others in the block for the planes, *i.e.* for the **k** vectors with two free parameters.

Table 1.5.5.4. *List of **k**-vector types for arithmetic crystal class $4/mmmI$: $c/a > 1$*

See Fig. 1.5.5.4. 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 |
|---|---|---|
| $\Gamma$ $0, 0, 0$ | 2 $a$ $4/mmm$ | $0, 0, 0$ |
| $M$ $\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}$ | 2 $b$ $4/mmm$ | $0, 0, \frac{1}{2}$ |
| $M \sim M_2$ | | $\frac{1}{2}, \frac{1}{2}, 0$ |
| $X$ $0, 0, \frac{1}{2}$ | 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 $f$ $..2/m$ | $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ |
| $\Lambda$ $\alpha, \alpha, -\alpha$ | 4 $e$ $4mm$ | $0, 0, z$: $0 < z < \frac{1}{2}$ |
| $W$ $\alpha, \alpha, \frac{1}{2} - \alpha$ | 8 $g$ $2mm.$ | $0, \frac{1}{2}, z$: $0 < z < \frac{1}{4}$ |
| $\Sigma$ $-\alpha, \alpha, \alpha$ | *ex* 8 $h$ $m.2m$ | $x, x, 0$: $0 < x \le s_2$ |
| $F$ $\frac{1}{2} - \alpha, \frac{1}{2} + \alpha, -\frac{1}{2} + \alpha$ | *ex* 8 $h$ $m.2m$ | $x, x, \frac{1}{2}$: $0 < x < s = \frac{1}{2} - s_2$ |
| $F \sim \Sigma_1 = [S_2\, M_2]$ | | $x, x, 0$: $s_2 < x < \frac{1}{2}$ |
| $\Sigma \cup \Sigma_1 = [\Gamma M_2]$ | 8 $h$ $m.2m$ | $x, x, 0$: $0 < x < \frac{1}{2}$ |
| $\Delta$ $0, 0, \alpha$ | 8 $i$ $m2m.$ | $0, y, 0$: $0 < y < \frac{1}{2}$ |
| $Y$ $-\alpha, \alpha, \frac{1}{2}$ | *ex* 8 $j$ $m2m.$ | $x, \frac{1}{2}, 0$: $0 < x \le r$ |
| $U$ $\frac{1}{2}, \frac{1}{2}, -\frac{1}{2} + \alpha$ | *ex* 8 $j$ $m2m.$ | $0, y, \frac{1}{2}$: $0 < y < g = \frac{1}{2} - r$ |
| $U \sim Y_1 = [R\, M_2]$ | | $x, \frac{1}{2}, 0$: $r < x < \frac{1}{2}$ |
| $Y \cup Y_1 = [X\, M_2]$ | 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 $k$ $..2$ | $x, \frac{1}{2} - x, \frac{1}{4}$: $0 < x < \frac{1}{4}$ |
| $C$ $-\alpha, \alpha, \beta$ | *ex* 16 $l$ $m..$ | $x, y, 0$: $[\Gamma\, S_2\, R\, X]$ |
| $D$ $\frac{1}{2} - \alpha, \frac{1}{2} + \alpha, -\frac{1}{2} + \beta$ | *ex* 16 $l$ $m..$ | $x, y, \frac{1}{2}$: $[M\, S\, G]$ |
| $D \sim C_1$ | | $x, y, 0$: $[M_2\, R\, S_2]$ |
| $C \cup C_1 = [\Gamma\, M_2\, X]$ | 16 $l$ $m..$ | $x, y, 0$: $0 < x < y < \frac{1}{2}$ |
| $B$ $\alpha, \beta, -\alpha$ | 16 $m$ $..m$ | $x, x, z$: $[\Gamma\, S_2\, S\, M]$ |
| $B = B_1 \cup B_2$ $= [\Gamma\, S_2\, N\, T] \cup [T\, N\, S\, M]$ | | |
| $B_2 \sim B_3$ | | $x, x, z$: $[T_2\, N\, S_2\, M_2]$ |
| $B_1 \cup B_3 = [\Gamma\, M_2\, T_2\, T]$ | 16 $m$ $..m$ | $x, x, z$: $0 < x < \frac{1}{2}, 0 < z < \frac{1}{4}$ $\cup$ $\cup$ $x, x, \frac{1}{4}$: $0 < x < \frac{1}{4}$ |
| $A$ $\alpha, \alpha, \beta$ | *ex* 16 $n$ $.m.$ | $0, y, z$: $[\Gamma\, X\, P\, G\, M]$ |
| $E$ $\alpha - \beta, \alpha + \beta, \frac{1}{2} - \alpha$ | *ex* 16 $n$ $.m.$ | $x, \frac{1}{2}, z$: $[X\, P\, R]$ |
| $E \sim A_1$ | | $0, y, z$: $[X_2\, G\, P]$ |
| $A \cup A_1 = [\Gamma\, X\, X_2\, M]$ | 16 $n$ $.m.$ | $0, y, z$: $0 < y, z < \frac{1}{2}$ |
| $GP$ $\alpha, \beta, \gamma$ | 32 $o$ $1$ | $x, y, z$: $0 < x < y < \frac{1}{2}; 0 < z < \frac{1}{4}$ $\cup$ $\cup$ $x, y, \frac{1}{4}$: $0 < x < y < \frac{1}{2} - x$ |

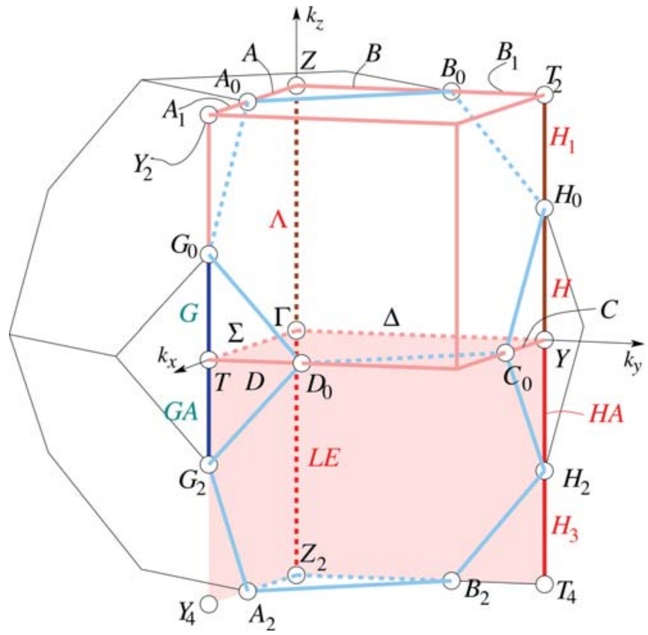


Fig. 1.5.5.5. Brillouin zone with asymmetric unit and representation domain of CDML for arithmetic crystal class $mm2F$: $a^{-2} < b^{-2} + c^{-2}$, $b^{-2} < c^{-2} + a^{-2}$ and $c^{-2} < a^{-2} + b^{-2}$. Space groups $Fmm2 - C_{2v}^{18}$ (42), $Fdd2 - C_{2v}^{19}$ (43). Reciprocal-space group $(Imm2)^*$, No. 44: $a^{*2} < b^{*2} + c^{*2}$, $b^{*2} < c^{*2} + a^{*2}$ and $c^{*2} < a^{*2} + b^{*2}$ (see Table 1.5.5.5). The representation domain of CDML is different from the asymmetric unit. Auxiliary points: $T_4$: $0, \frac{1}{2}, -\frac{1}{2}$; $Y_2$: $\frac{1}{2}, 0, \frac{1}{2}$; $Y_4$: $\frac{1}{2}, 0, -\frac{1}{2}$; $Z_2$: $0, 0, -\frac{1}{2}$. 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 1.5.5.5. *List of* **k***-vector types for arithmetic crystal class* $mm2F$: $a^{-2} < b^{-2} + c^{-2}$, $b^{-2} < c^{-2} + a^{-2}$ *and* $c^{-2} < a^{-2} + b^{-2}$

See Fig. 1.5.5.5. 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 |
|---|---|---|
| $\Gamma$ $0, 0, 0$ | *ex* 2 *a* *mm*2 | $0, 0, 0$ |
| $Z$ $\frac{1}{2}, \frac{1}{2}, 0$ | *ex* 2 *a* *mm*2 | $0, 0, \frac{1}{2}$ |
| $\Lambda$ $\alpha, \alpha, 0$ | *ex* 2 *a* *mm*2 | $0, 0, z$: $0 < z < \frac{1}{2}$ |
| $LE$ $-\alpha, -\alpha, 0$ | *ex* 2 *a* *mm*2 | $0, 0, z$: $-\frac{1}{2} < z < 0$ |
| $\Gamma \cup \Lambda \cup Z \cup LE$ | 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 | $\frac{1}{2}, 0, z$: $0 < z \le g_0$ |
| $G \sim H_3 = [H_2\, T_4]$ | | $0, \frac{1}{2}, z$: $-\frac{1}{2} < z \le -\frac{1}{2} + g_0 = h_2$ |
| $GA$ $-\alpha, \frac{1}{2} - \alpha, \frac{1}{2}$ | *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 | $0, \frac{1}{2}, z$: $-\frac{1}{2} < z \le \frac{1}{2}$ |
| $\Sigma$ $0, \alpha, \alpha$ | *ex* 4 *c* *.m.* | $x, 0, 0$: $0 < x < \frac{1}{2}$ |
| $A$ $\frac{1}{2}, \frac{1}{2} + \alpha, \alpha$ | *ex* 4 *c* *.m.* | $x, 0, \frac{1}{2}$: $0 < x \le a_0$ |
| $C$ $\frac{1}{2}, \alpha, \frac{1}{2} + \alpha$ | *ex* 4 *c* *.m.* | $x, \frac{1}{2}, 0$: $0 < x < c_0 = \frac{1}{2} - a_0$ |
| $C \sim A_1$ | | $x, 0, \frac{1}{2}$: $\frac{1}{2} - a_0 = c_0 < x < \frac{1}{2}$ |
| $J$ $\alpha, \alpha + \beta, \beta$ | *ex* 4 *c* *.m.* | $x, 0, z$: $[\Gamma\, Z\, A_0\, G_0\, T]$ |
| $JA$ $-\alpha, -\alpha + \beta, \beta$ | *ex* 4 *c* *.m.* | $x, 0, z$: $[\Gamma\, T\, G_2\, A_2\, Z_2]$ |
| $K$ $\frac{1}{2} + \alpha, \alpha + \beta, \frac{1}{2} + \beta$ | *ex* 4 *c* *.m.* | $x, \frac{1}{2}, z$: $[Y\, H_0\, C_0]$ |
| $K \sim J_1$ | | $x, 0, z$: $[Y_4\, G_2\, A_2]$ |
| $KA$ $\frac{1}{2} - \alpha, -\alpha + \beta, \frac{1}{2} + \beta$ | *ex* 4 *c* *.m.* | $x, \frac{1}{2}, z$: $[Y\, C_0\, H_2]$ |
| $KA \sim J_3$ | | $x, 0, z$: $[Y_2\, G_0\, A_0]$ |
| $A \cup A_1 \cup J \cup J_3 \cup \Sigma \cup JA \cup J_1$ | 4 *c* *.m.* | $x, 0, z$: $0 < x < \frac{1}{2}$; $0 < z \le \frac{1}{2}$ |
| $\Delta$ $\alpha, 0, \alpha$ | *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..* | $0, y, \frac{1}{2}$: $0 < y < b_0$ |
| $D$ $\alpha, \frac{1}{2}, \frac{1}{2} + \alpha$ | *ex* 4 *d* *m..* | $\frac{1}{2}, y, 0$: $0 < y \le d_0$ |
| $D \sim B_1$ | | $0, y, \frac{1}{2}$: $\frac{1}{2} - d_0 = b_0 \le y < \frac{1}{2}$ |
| $E$ $\alpha + \beta, \alpha, \beta$ | *ex* 4 *d* *m..* | $0, y, z$: $[\Gamma\, Y\, H_0\, B_0\, Z]$ |
| $EA$ $-\alpha + \beta, -\alpha, \beta$ | *ex* 4 *d* *m..* | $0, y, z$: $[\Gamma\, Z_2\, B_2\, H_2\, Y]$ |
| $F$ $\alpha + \beta, \frac{1}{2} + \alpha, \frac{1}{2} + \beta$ | *ex* 4 *d* *m..* | $\frac{1}{2}, y, z$: $[T\, D_0\, G_0]$ |
| $F \sim E_3$ | | $0, y, z$: $[B_2\, T_4\, H_2]$ |
| $FA$ $-\alpha + \beta, \frac{1}{2} - \alpha, \frac{1}{2} + \beta$ | *ex* 4 *d* *m..* | $\frac{1}{2}, y, z$: $[T\, G_2\, D_0]$ |
| $FA \sim E_1$ | | $0, y, z$: $[T_2\, B_0\, H_0]$ |
| $\Delta \cup B \cup B_1 \cup E \cup E_1 \cup EA \cup E_3$ | 4 *d* *m..* | $0, y, z$: $0 < y < \frac{1}{2}$; $-\frac{1}{2} < z \le \frac{1}{2}$ |
| $GP$ $\alpha, \beta, \gamma$ | 8 *e* 1 | $x, y, z$: $0 < x, y < \frac{1}{2}$; $0 < z \le \frac{1}{2}$ |

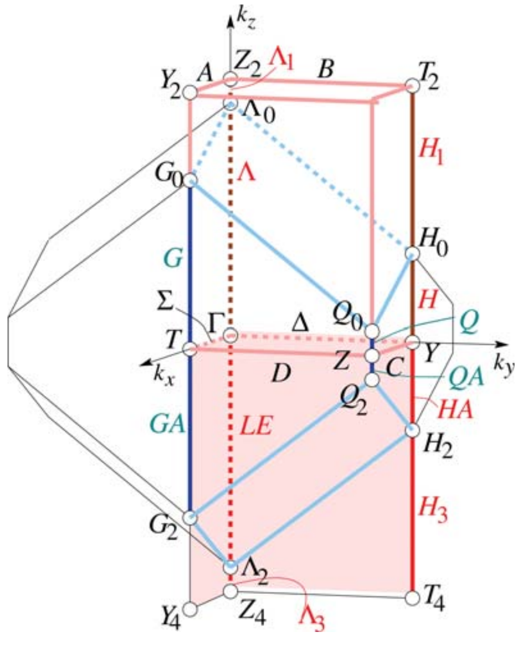


Fig. 1.5.5.6. Brillouin zone with asymmetric unit and representation domain of CDML for arithmetic crystal class *mm2F*: $c^{-2} > a^{-2} + b^{-2}$. Space groups $Fmm2 - C_{2v}^{18}$ (42), $Fdd2 - C_{2v}^{19}$ (43). Reciprocal-space group (*Imm*2)*, No. 44: $c^{*2} > a^{*2} + b^{*2}$ (see Table 1.5.5.6).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

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:

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

instead of

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

### 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.

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 |
|---|---|---|
| $\Gamma$ $0, 0, 0$ | *ex* 2 *a* *mm*2 | $0, 0, 0$ |
| $Z$ $\frac{1}{2}, \frac{1}{2}, 1$ | *ex* 2 *a* *mm*2 | $\frac{1}{2}, \frac{1}{2}, 0$ |
| $Z \sim Z_2$ | | $0, 0, \frac{1}{2}$ |
| $\Lambda$ $\alpha, \alpha, 0$ | *ex* 2 *a* *mm*2 | $0, 0, z$: $0 < z \leq \lambda_0$ |
| $LE$ $-\alpha, -\alpha, 0$ | *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 | $\frac{1}{2}, \frac{1}{2}, z$: $0 < z \leq q_0$ |
| $Q \sim \Lambda_3 = [\Lambda_2\, Z_4]$ | | $0, 0, z$: $-\frac{1}{2} < z \leq -\frac{1}{2} + q_0 = -\lambda_0$ |
| $QA$ $\frac{1}{2} - \alpha, \frac{1}{2} - \alpha, 1$ | *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 | $0, 0, z$: $-\frac{1}{2} < z \leq \frac{1}{2}$ |
| $T$ $0, \frac{1}{2}, \frac{1}{2}$ | *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 | $\frac{1}{2}, 0, z$: $0 < z \leq g_0$ |
| $G \sim H_3 = [H_2\, T_4]$ | | $0, \frac{1}{2}, z$: $-\frac{1}{2} < z \leq -\frac{1}{2} + g_0$ |
| $GA$ $-\alpha, \frac{1}{2} - \alpha, \frac{1}{2}$ | *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 | $0, \frac{1}{2}, z$: $0 < z \leq h_0$ |
| $HA$ $\frac{1}{2} - \alpha, -\alpha, \frac{1}{2}$ | *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 | $0, \frac{1}{2}, z$: $-\frac{1}{2} < z \leq \frac{1}{2}$ |
| $\Sigma$ $0, \alpha, \alpha$ | *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*. | $x, 0, z$: $0 < x < \frac{1}{2}$; $-\frac{1}{2} < z \leq \frac{1}{2}$ |
| $\Delta$ $\alpha, 0, \alpha$ | *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*.. | $0, y, z$: $0 < y < \frac{1}{2}$; $-\frac{1}{2} < z \leq \frac{1}{2}$ |
| $GP$ $\alpha, \beta, \gamma$ | 8 *e* 1 | $x, y, z$: $0 < x, y < \frac{1}{2}$; $0 < z \leq \frac{1}{2}$ |

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



references