International Tables for Crystallography (2010). Vol. B, Section 1.5.5, pp. 181–191.

Table 1.5.4.1. *Conventional coefficients* $(k_i)^T$ *of* **k** *expressed by the adjusted coefficients* (k_{ai}) *of IT A for the different Bravais types of lattices in direct space*

Lattice types	k_1	k_2	k_3
aP, *mP*, *oP*, *tP*, *cP*, *rP*	k_{a1}	k_{a2}	k_{a3}
mA, *oA*	k_{a1}	$2k_{a2}$	$2k_{a3}$
mC, *oC*	$2k_{a1}$	$2k_{a2}$	k_{a3}
oF, *cF*, *oI*, *cI*	$2k_{a1}$	$2k_{a2}$	$2k_{a3}$
tI	$k_{a1} + k_{a2}$	$-k_{a1} + k_{a2}$	$2k_{a3}$
hP	$k_{a1} - k_{a2}$	k_{a2}	k_{a3}
hR (hexagonal)	$2k_{a1} - k_{a2}$	$-k_{a1} + 2k_{a2}$	$3k_{a3}$

Table 1.5.4.2. *Primitive coefficients* $(k_{pi})^T$ *of* **k** *from CDML expressed by the adjusted coefficients* (k_{ai}) *of IT A for the different Bravais types of lattices in direct space*

Lattice types	k_{p1}	k_{p2}	k_{p3}
aP, *mP*, *oP*, *tP*, *cP*, *rP*	k_{a1}	k_{a2}	k_{a3}
mA, *oA*	k_{a1}	$k_{a2}-k_{a3}$	$k_{a2}+k_{a3}$
mC, *oC*	$k_{a1}-k_{a2}$	$k_{a1}+k_{a2}$	k_{a3}
oF, *cF*	$k_{a2}+k_{a3}$	$k_{a1}+k_{a3}$	$k_{a1}+k_{a2}$
oI, *cI*	$-k_{a1}+k_{a2}+k_{a3}$	$k_{a1}-k_{a2}+k_{a3}$	$k_{a1}+k_{a2}-k_{a3}$
tI	$-k_{a1}+k_{a3}$	$k_{a1}+k_{a3}$	$k_{a2}-k_{a3}$
hP	$k_{a1}-k_{a2}$	k_{a2}	k_{a3}
hR (hexagonal)	$k_{a1}+k_{a3}$	$-k_{a1}+k_{a2}+k_{a3}$	$-k_{a2}+k_{a3}$

irreps belonging to a **k** vector are specified by these parameters and the irreps belonging to a **k**-vector type form a *type of irreps*, Boyle (1986).

It may be advantageous to describe the different stars belonging to a Wintgen position in a *uniform* way. For this purpose one can define:

Definition. Two **k** vectors of a Wintgen position are *uni-arm* if one can be obtained from the other by parameter variation. The *description of the stars* of a Wintgen position is *uni-arm* if the **k** vectors representing these stars are uni-arm.

The uni-arm description is particularly useful to check whether different sets of **k** vectors belong to the same **k**-vector type or not. Because of the shape of the representation domain or of the asymmetric unit, a **k**-vector type may be split into different parts which belong to different arms of different **k**-vector stars. A uni-arm description may be obtained by the introduction of flagpoles and wings, see Section 1.5.5.1.

For the uni-arm description of a Wintgen position it is easy to check whether the parameter ranges for the general or special constituents of the representation domain or asymmetric unit have been stated correctly. For this purpose one may define the *field of* **k** as the parameter space (point, line, plane or space) of a Wintgen position. For the check one determines that part of the field of **k** which is in the unit cell. The order of the little co-group $\overline{\mathcal{G}}^{\mathbf{k}}$ ($\overline{\mathcal{G}}^{\mathbf{k}}$ represents those operations which leave the field of **k** *fixed pointwise*) is divided by the order of the stabilizer of the field in $(\mathcal{G})^*$ [which is the set of all symmetry operations mod (integer translations) which leave the field *invariant as a whole*]. The result gives the independent fraction of the volume of the unit cell or the area of the plane or length of the line.

If the description is not uni-arm, the uni-arm parameter range will be split into the parameter ranges of the different arms. These parameter ranges of the different arms are not necessarily equal, for examples see Section 1.5.5.

Remark. One should avoid the term *equivalent* for the relation between **k** vectors of the same type but with different parameters, as used by Stokes *et al.* (1993) for Λ and *F* or *B*, *C* and *J* of $m\overline{3}mI$, see examples (1) and (2) in Section 1.5.5.4.4. To belong to the same **k**-vector type is only a necessary, not a sufficient, condition for **k**-vector equivalence. On p. 95 of BC is the following definition: 'Two **k** vectors $\mathbf{k}_1$ and $\mathbf{k}_2$ are equivalent if $\mathbf{k}_1 = \mathbf{k}_2 + \mathbf{K}$, where $\mathbf{K} \in \mathbf{L}^*$'. One can express this by saying: 'Two **k** vectors are equivalent if their difference is a vector **K** of the (reciprocal) lattice'. We prefer to extend this equivalence by saying: 'Two **k** vectors $\mathbf{k}_1$ and $\mathbf{k}_2$ are equivalent if and only if they belong to the same orbit of **k**', *i.e* if there is a matrix part *W* and a vector $\mathbf{K} \in \mathbf{L}^*$ belonging to $\mathcal{G}$ such that $\mathbf{k}_2 = \mathbf{W}\mathbf{k}_1 + \mathbf{K}$, see equation (1.5.3.13). The **k** vectors of Stokes *et al.* (1993) are not equivalent under this definition, see Davies & Dirl (1987). If the representatives of the **k**-vector stars are chosen uni-arm, their non-equivalence is evident.

It must be mentioned that two **k** vectors of the same type are only called equivalent here if they belong to the same *orbit* of **k** vectors, *i.e.* a **k**-vector type is *not* an equivalence class with respect to the definition of equivalence stated in this remark.

There are two main reasons why **k** vectors of the same type split and then have different labels in CDML:

(1) The higher the symmetry of the point group $\overline{\mathcal{G}}$ of $\mathcal{G}$, the higher is the symmetry of the lattice $\mathbf{L}(\mathcal{G})$ and of the reciprocal lattice $\mathbf{L}^*$, and thus of the Brillouin zone of $\mathcal{G}$. As the symmetry of the Brillouin zone increases, the choice of the boundaries of the representation domain and any other minimal domain becomes more and more restricted. This is because a symmetry element (rotation or rotoinversion axis, plane of reflection, centre of inversion) cannot occur in the interior of the minimal domain but only on its boundary. For the arithmetic crystal class $m\overline{3}mI$, for example, all boundary planes, lines and points are fixed, such that all possible minimal domains are equivalent.

For lower point-group symmetries of the fundamental regions, the choice of the minimal domain is less restricted but the Brillouin zones may become more complicated and may even belong to different topological types depending on the ratios of the lattice parameters. Faces and lines on the surface of the Brillouin zone may appear or disappear or change their relative sizes depending on the lattice parameters, causing different descriptions of Wintgen positions.

This does not happen in unit cells or their asymmetric units. Therefore, as already mentioned in Section 1.5.4.1, BC and CDML preferred to replace the different complicated bodies of the Brillouin zones for the possible values of the lattice parameters of the triclinic and monoclinic lattices by the simple primitive unit cells of the reciprocal lattice and to choose the representation domain correspondingly.

(2) For non-holosymmetric space groups the representation domain Φ is a multiple of the basic domain Ω. CDML introduce new letters for **k** vectors which do not belong to Ω. The more symmetry a space group has lost compared to its holosymmetric space group, the more letters of **k** vectors are introduced. The symbols of the basic domain Ω are kept in the names referred to the representation domain Φ. In most cases one can make the new **k** vectors uni-arm to **k** vectors of the basic domain Ω by an appropriate choice of Ω and Φ. Then these **k** vectors belong to the same **k**-vector type and the additional labels can be avoided by *extension of the parameter range* in the **k**-vector space (Boyle, 1986).

Examples where new letters can be avoided by the extension of the parameter range are common, see, *e.g.*, the examples of Section 1.5.5.

In the following example, the introduction of a new name in the transition from a holosymmetric space group to a non-holosymmetric one cannot be avoided because the Wintgen position splits into two positions. We consider the **k** label *Z*, $\alpha, \frac{1}{2}, 0$ of CDML for the arithmetic crystal class $m\overline{3}mP$, reciprocal-space group $(\mathcal{G})^* = (Pm\overline{3}m)^*$, isomorphic to $Pm\overline{3}m$, Wyckoff position 12 *h* *mm*2 $x, \frac{1}{2}, 0$. In the subgroup $(Pm\overline{3})^*$, this Wintgen position splits into the two positions $\alpha, \frac{1}{2}, 0$ and $\frac{1}{2},\alpha,0$, called *Z* and *ZA* by CDML. In the description of *IT* A they are 6 *g* *mm*2 $x, \frac{1}{2}, 0$ and 6 *f* *mm*2 $\frac{1}{2}, x, 0$. In $Pm\overline{3}$, they form two different Wyckoff positions and thus need two different names, as do their Wintgen positions.

1.5.5. Examples and discussion

The comparison of the crystallographic classification scheme with the traditional one is illustrated by four examples from the Bilbao Crystallographic Server (1998). The examples are designated by the arithmetic crystal classes.

To each arithmetic crystal class of space groups, *cf.* Section 1.5.3.2, there belongs exactly one reciprocal-space group $(\mathcal{G})^*$ which is isomorphic to a type of symmorphic space groups $\mathcal{G}_0$, *cf.* Sections 1.5.3.2 and 1.5.3.4.

(1) **k**-vector types of the arithmetic crystal class $m\bar{3}mI$ (space groups $Im\bar{3}m$ and $Ia\bar{3}d$), reciprocal-space group $(\mathcal{G})^*$ isomorphic to $Fm\bar{3}m$. The representation domain $\Phi = \Omega$ is equal to the asymmetric unit, see Fig. 1.5.5.1 and Table 1.5.5.1.

(2) **k**-vector types of the arithmetic crystal class $m\bar{3}I$ (space groups $Im\bar{3}$ and $Ia\bar{3}$), reciprocal-space group $(\mathcal{G})^*$ isomorphic to $Fm\bar{3}$. The representation domain $\Phi > \Omega$ is equal to the asymmetric unit; see Fig. 1.5.5.2 and Table 1.5.5.2.

(3) **k**-vector types of the arithmetic crystal class $4/mmmI$ ($I4/mmm$, $I4/mcm$, $I4_1/amd$ and $I4_1/acd$), reciprocal-space group $(\mathcal{G})^*$ isomorphic to $I4/mmm$. The representation domains $\Phi = \Omega$ are topologically different for different ratios of the lattice parameters a and c whereas the asymmetric units are affinely equivalent; see Figs. 1.5.5.3 and 1.5.5.4 and Tables 1.5.5.3 and 1.5.5.4.

(4) **k**-vector types of the arithmetic crystal class $mm2F$ ($Fmm2$ and $Fdd2$), reciprocal-space group $(\mathcal{G})^*$ isomorphic to $Imm2$. The representation domains $\Phi > \Omega$ are topologically different for different ratios of the lattice parameters a, b and c whereas the asymmetric units are affinely equivalent; see Figs. 1.5.5.5, 1.5.5.6 and 1.5.5.7, and Tables 1.5.5.5, 1.5.5.6 and 1.5.5.7.

These examples consist essentially of figures and tables. The Brillouin zones with the representation domains of CDML together with the asymmetric units are displayed in the figures. In the synoptic tables the correlation between the **k**-vector tables of CDML and the tables of (Wyckoff) positions in *IT* A is presented. One can thus compare the different descriptions and recognize the relations between them. In addition, the parameter ranges of the **k**-vector types in the asymmetric unit are stated. If a **k**-vector type is listed in the table more than once, then the equivalence relations between the **k** vectors are added such that exactly one representative may be selected for each **k**-vector orbit.

1.5.5.1. Guide to the figures

Each figure caption gives the name of the arithmetic crystal class of space groups to which the Brillouin zone belongs. If there is more than one figure for this arithmetic crystal class, then these figures refer to different geometric conditions for the lattice. Therefore, for each of the figures the arithmetic crystal class is followed by the specific conditions for the lattice parameters of this figure, *e.g.* '$c/a < 1$' for Fig. 1.5.5.3 or '$a^{-2} < b^{-2} + c^{-2}$, $b^{-2} < c^{-2} + a^{-2}$ and $c^{-2} < a^{-2} + b^{-2}$' for Fig. 1.5.5.5.

Then the space groups of the arithmetic crystal class are listed with their Hermann–Mauguin symbols, their Schoenflies symbols and their space-group numbers in *IT* A in parentheses. Following this the type of the reciprocal-space group is denoted, *e.g.* '$(Imm2)^*$, No. 44' for the arithmetic crystal class $mm2F$ in Fig. 1.5.5.5, together with the conditions for the lattice parameters of the reciprocal lattice, if any, and the number of the corresponding table.

The Brillouin zones are objects in reciprocal space. They are displayed in the figures. The reciprocal space is a vector space and its elements are the **k** vectors. Thus the Brillouin zone is a construction in vector space. Because the Brillouin zones are visualized by drawings consisting of vertices, lines and planes, one usually speaks of points, lines and planes in or on the border of the Brillouin zone, not of vectors. Here we follow this tradition.

The Brillouin zones are projected onto the drawing plane by a clinographic projection which may be found *e.g.* in Smith (1982), pp. 61 *f.* The coordinate axes are designated k_x, k_y and k_z; the k_z-coordinate axis points upwards in the projection plane. The diagrams of the Brillouin zones follow those of CDML in order to facilitate the comparison of the data. The origin O with coordinates 0, 0, 0 always forms the centre of the Brillouin zone and is called Γ.

A minimal domain is the smallest fraction of the Brillouin zone which contains *exactly* one wavevector **k** from each orbit. In these examples, the representation domain of CDML is compared with the minimal domain, called 'asymmetric unit', of the Bilbao Crystallographic Server. This asymmetric unit is a simple body and is often chosen in analogy to that of *IT* A. It may coincide with the representation domain of Table 3.10 in CDML, but is mostly rather different. Other than the representation domains of CDML, the asymmetric unit is often *not* fully contained in the Brillouin zone but protrudes from it, in particular by flagpoles and wings, *cf.* the end of this section.

In the figures the edges of the chosen asymmetric unit are drawn into the frame of the Brillouin zone. The names of points, lines and planes of CDML are retained in this listing. New names have been given to points and lines which are not listed in CDML.

The shape of the Brillouin zone depends on the lattice relations. Therefore, there may be vertices of the Brillouin zone with a variable coordinate. If such a point is displayed and designated in a figure by an upper-case letter, then the label of its variable coordinate in the corresponding table is the same letter but lower case. Thus, the variable coordinate of the point G_0 is g_0, of Λ_0 is λ_0 *etc.*

In CDML, the same letter may designate items of different quality in different figures and tables. For example, there is a point H in Fig. 1.5.5.1 and Table 1.5.5.1 but a line H in Fig. 1.5.5.5 and Table 1.5.5.5. In the figures and tables of these examples not only lines and points but also their equivalent objects are listed and the parameter ranges of the lines are described. Therefore, the endpoints of the line H, the points equivalent to a point H as well as the lines equivalent to a line H may be also designated by the letter H but distinguished by indices. In order to recognize points and lines easily, the indices of points are always even: H_0, H_2, H_4; those of lines are always odd: H_1, H_3.

A point is marked in a figure by its name and by a black circle filled with white if it is listed in the corresponding **k**-vector table but is not a point of special symmetry. The same designation is used for the auxiliary points that have been added in order to facilitate the comparison between the two descriptions of the **k**-vector types. Non-coloured parts of the coordinate axes, of the edges of the Brillouin zone or auxiliary lines are displayed by thin solid black lines. Such lines are dashed or omitted if they are not visible, *i.e.* are hidden by the body of the Brillouin zone or of the asymmetric unit.

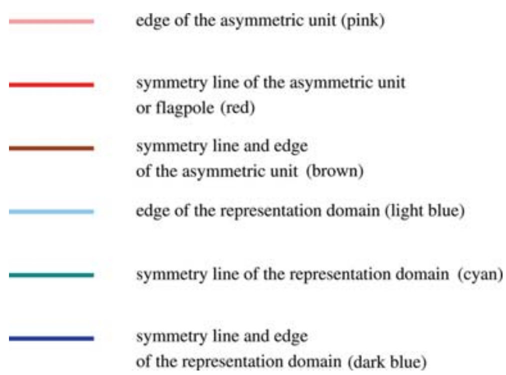
The representatives for the orbits of symmetry points or of symmetry lines, as well as the edges of the representation domain of CDML and of the chosen asymmetric unit are shown in colour.

(*a*) A representative point of each orbit of symmetry points is designated by a red- or cyan-filled circle with its name also in red or cyan if it belongs to the asymmetric unit or to the representation domain of CDML. If both colours could be used, *e.g.* if the asymmetric unit coincides with the representation domain, the colour is red.

Note that a point is coloured red or cyan only if it is really a symmetry *point*, *i.e.* its little co-group is a proper supergroup of the little co-groups of all points in its neighbourhood. Such a point has no variable parameters in its coordinates. Points listed by CDML are not coloured if they are part of a symmetry line or symmetry plane only.

(*b*) Coloured lines are always broad. They are solid lines if they are 'visible', *i.e.* if they are not hidden by the Brillouin zone or by the asymmetric unit. A hidden symmetry line or edge of the asymmetric unit is not suppressed but is coloured as a *dashed line*.

(*c*) The meanings of the different coloured lines and the names used for them in the text are as follows:



Notes:

(1) The colour of the line is pink for an edge of the asymmetric unit which is not a symmetry line.

(2) The colour is red for a symmetry line of the asymmetric unit, with the name also in red.

(3) The colour of the line is brown with the name in red for a line which is a symmetry line as well as an edge of the asymmetric unit.

The representation domain of CDML is displayed in the same figure.

(1) The edges of the representation domain are coloured light blue.

(2) The symmetry points and lines with their letters are coloured cyan.

(3) Edges of the representation domain or common edges of the representation domain and the asymmetric unit are coloured dark blue with the letters in cyan if they are symmetry lines of the representation domain but not of the asymmetric unit.

Common edges of an asymmetric unit and a representation domain are coloured pink if they are not symmetry lines simultaneously.

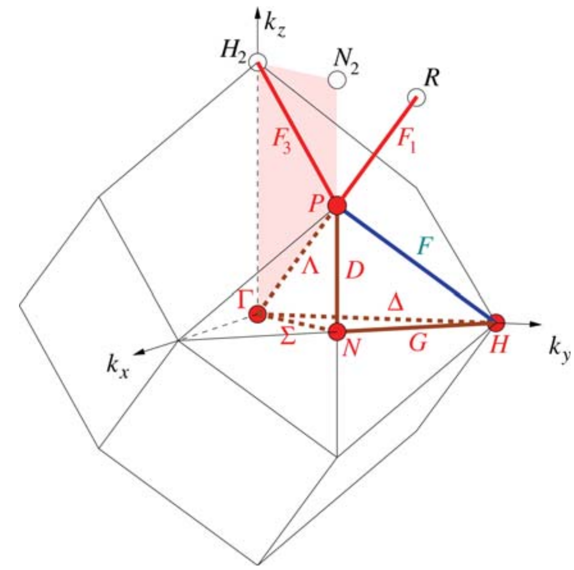


Fig. 1.5.5.1. Brillouin zone with asymmetric unit and representation domain of CDML for arithmetic crystal class $m\bar{3}mI$. Space groups: $Im\bar{3}m - O_h^9$ (229), $Ia\bar{3}d - O_h^{10}$ (230). Reciprocal-space group $(Fm\bar{3}m)$*, No. 225 (see Table 1.5.5.1). The representation domain of CDML is identical with the asymmetric unit. Auxiliary points: R: $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$; N_2: $\frac{1}{4}, \frac{1}{4}, \frac{1}{2}$; H_2: $0, 0, \frac{1}{2}$. Flagpole: $F_1 = [P\,R]$ x, x, x: $\frac{1}{4} < x < \frac{1}{2}$. Wing: $B_1 \cup J_1 = [\Gamma\,P\,N_2\,H_2] \backslash [F_3]$ x, x, z: $0 < x < \frac{1}{4}$; $x < z < \frac{1}{2}$ with $z \neq \frac{1}{2} - x$.

Exactly one element of each point orbit, line orbit or orbit of planes is contained in the asymmetric unit. Exceptionally, *different* elements of the *same* orbit have been coloured because of their special meaning. In these cases the different elements are connected in the corresponding table by the equivalence sign $\sim$, see, *e.g.* the lines $F \sim F_1 = [P\,R]$ or the planes $B \sim B_1 = [P\,N_2\,H_2]$ in Table 1.5.5.1.

To enable a uni-arm description, symmetry lines outside the asymmetric unit may be selected as orbit representatives. Such a piece of a line is called a *flagpole*. Flagpoles are always coloured red, see, *e.g.*, the line F_1 in Fig. 1.5.5.1.

Symmetry planes are not distinguished in the figures. However, in analogy to the flagpoles, symmetry planes outside the asym-

Table 1.5.5.1. *List of* **k***-vector types for arithmetic crystal class* $m\bar{3}mI$

See Fig. 1.5.5.1. Parameter relations: $x = \frac{1}{2}\beta + \frac{1}{2}\gamma$, $y = \frac{1}{2}\alpha + \frac{1}{2}\gamma$, $z = \frac{1}{2}\alpha + \frac{1}{2}\beta$.

k-vector label, CDML	Wyckoff position of *IT* A, *cf.* Section 1.5.4.3	Parameters
Γ $0, 0, 0$	4 a $m\bar{3}m$	$0, 0, 0$
H $\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}$	4 b $m\bar{3}m$	$0, \frac{1}{2}, 0$
P $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	8 c $\bar{4}3m$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$
N $0, 0, \frac{1}{2}$	24 d $m.mm$	$\frac{1}{4}, \frac{1}{4}, 0$
Δ $\alpha, -\alpha, \alpha$	24 e $4m.m$	$0, y, 0$: $0 < y < \frac{1}{2}$
Λ α, α, α	*ex* 32 f $.3m$	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 $.3m$	$x, \frac{1}{2} - x, x$: $0 < x < \frac{1}{4}$
$F \sim F_1 = [P\,R]$		x, x, x: $\frac{1}{4} < x < \frac{1}{2}$
$F \sim F_3 = [P\,H_2]$		$x, x, \frac{1}{2} - x$: $0 < x < \frac{1}{4}$
$\Lambda \cup F_1 = [\Gamma R] \backslash [P]$	32 f $.3m$	x, x, x: $0 < x < \frac{1}{2}, x \neq \frac{1}{4}$
D $\alpha, \alpha, \frac{1}{2} - \alpha$	48 g $2.mm$	$\frac{1}{4}, \frac{1}{4}, z$: $0 < z < \frac{1}{4}$
Σ $0, 0, \alpha$	48 h $m.m2$	$x, x, 0$: $0 < x < \frac{1}{4}$
G $\frac{1}{2} - \alpha, -\frac{1}{2} + \alpha, \frac{1}{2}$	48 i $m.m2$	$x, \frac{1}{2} - x, 0$: $0 < x < \frac{1}{4}$
A $\alpha, -\alpha, \beta$	96 j $m..$	$x, y, 0$: $0 < x < y < \frac{1}{2} - x$
B $\alpha + \beta, -\alpha + \beta, \frac{1}{2} - \beta$	*ex* 96 k $..m$	$x, \frac{1}{2} - x, z$: $0 < z < x < \frac{1}{4}$
$B \sim B_1 = [P\,N_2\,H_2]$		x, x, z: $0 < x < \frac{1}{2} - x < z < \frac{1}{2}$
C α, α, β	*ex* 96 k $..m$	x, x, z: $0 < z < x < \frac{1}{4}$
J α, β, α	*ex* 96 k $..m$	x, y, x: $0 < x < y < \frac{1}{2} - x$
$J \sim J_1 = [\Gamma\,P\,H_2]$		x, x, z: $0 < x < z < \frac{1}{2} - x$
$C \cup B_1 \cup J_1 = [\Gamma\,N\,N_2\,H_2] \backslash [\Lambda, F_3]$	96 k $..m$	x, x, z: $0 < x < \frac{1}{4}, 0 < z < \frac{1}{2}$ with $z \neq x, z \neq \frac{1}{2} - x$
GP α, β, γ	192 l 1	x, y, z: $0 < z < x < y < \frac{1}{2} - x$

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 '∼' 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.

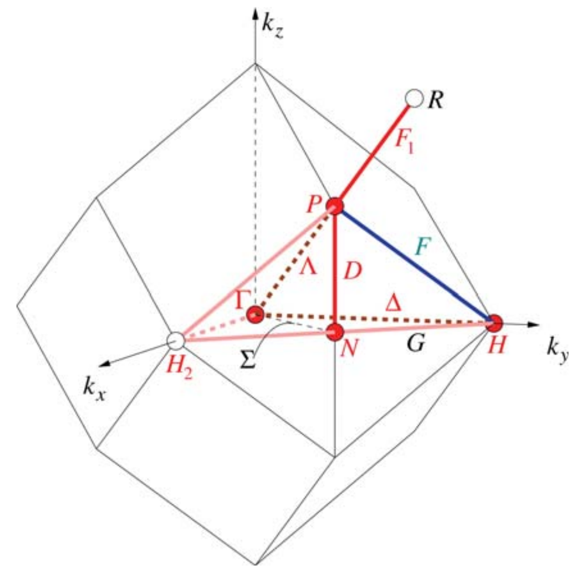


Fig. 1.5.5.2. Brillouin zone with asymmetric unit and representation domain of CDML for arithmetic crystal class $m\bar{3}I$. Space groups $Im\bar{3}-T_h^5$ (204), $Ia\bar{3}-T_h^7$ (206). Reciprocal-space group $(Fm\bar{3})$*, No. 202 (see Table 1.5.5.2). The representation domain of CDML is identical 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
Γ 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* $2/m..$	$\frac{1}{4}, \frac{1}{4}, 0$
Δ $\alpha, -\alpha, \alpha$	24 *e* $mm2..$	$0, y, 0$: $0 < y < \frac{1}{2}$
Λ α, α, α	*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..	$\frac{1}{4}, \frac{1}{4}, z$: $0 < z < \frac{1}{4}$
Σ $0, 0, \alpha$	*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* $m..$	$x, y, 0$: $0 < y < \frac{1}{2}-x < \frac{1}{2}$ ∪ ∪ $x, \frac{1}{2}-x, 0$: $0 < x < \frac{1}{4}$
GP α, β, γ	96 *i* 1	x, y, z: $0 < z \leq x < y < \frac{1}{2}-x$ ∪ ∪ x, y, z: $0 < z < y < x \leq \frac{1}{2}-y$ ∪ ∪ x, x, z: $0 < z < x < \frac{1}{4}$

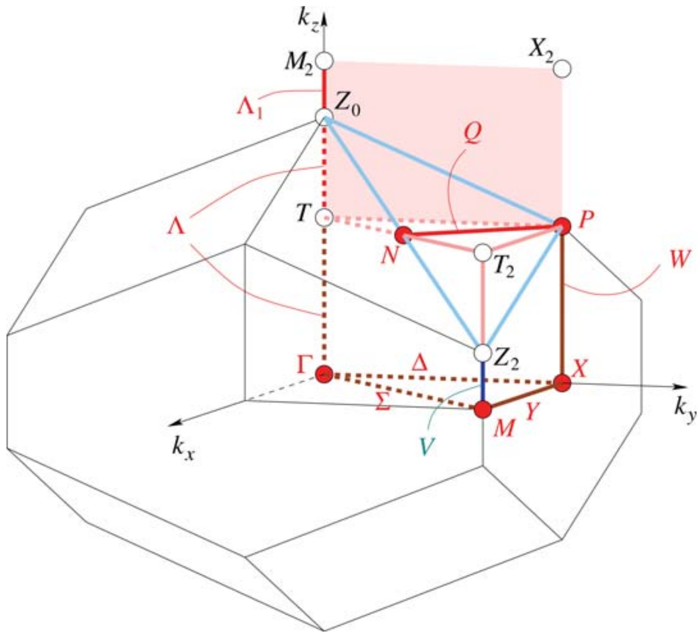


Fig. 1.5.5.3. Brillouin zone with asymmetric unit and representation domain of CDML for arithmetic crystal class $4/mmmI$: $c/a < 1$. Space groups $I4/mmm - D_{4h}^{17}$ (139) to $I4_1/acd - D_{4h}^{20}$ (142). Reciprocal-space group $(I4/mmm)^*$, No. 139: $c^*/a^* > 1$ (see Table 1.5.5.3). The representation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

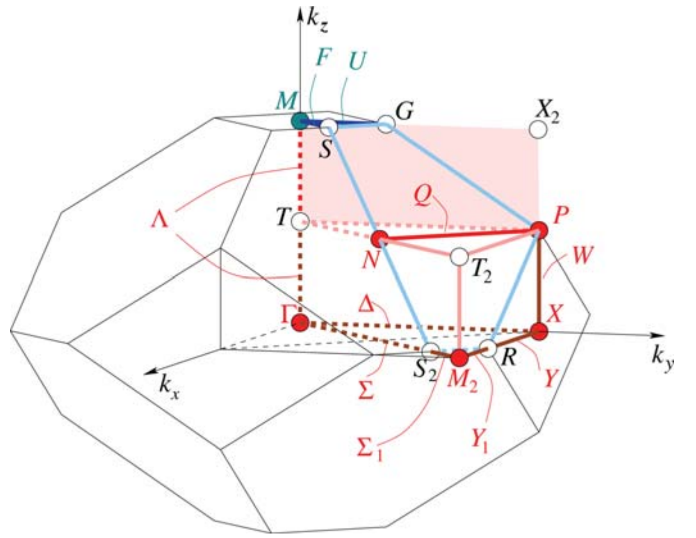


Fig. 1.5.5.4. Brillouin zone with asymmetric unit and representation domain of CDML for arithmetic crystal class $4/mmmI$: $c/a > 1$. Space groups $I4/mmm - D_{4h}^{17}$ (139) to $I4_1/acd - D_{4h}^{20}$ (142). Reciprocal-space group $(I4/mmm)^*$, No. 139: $c^*/a^* < 1$ (see Table 1.5.5.4). The representation 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 'Γ $0, 0, 0$' 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, Γ and Z are listed together with 'Λ $\alpha, \alpha, 0$' 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 'Σ $0, \alpha, \alpha$' 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, Σ 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
Γ $0, 0, 0$	2 a $4/mmm$	$0, 0, 0$
M $\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}$	2 b $4/mmm$	$0, 0, \frac{1}{2}$
$M \sim M_2$		$\frac{1}{2}, \frac{1}{2}, 0$
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 $..2/m$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$
Λ $\alpha, \alpha, -\alpha$	4 e $4mm$	$0, 0, z$: $0 < z < \frac{1}{2}$
W $\alpha, \alpha, \frac{1}{2} - \alpha$	8 g $2mm.$	$0, \frac{1}{2}, z$: $0 < z < \frac{1}{4}$
Σ $-\alpha, \alpha, \alpha$	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 $m.2m$	$x, x, 0$: $0 < x < \frac{1}{2}$
Δ $0, 0, \alpha$	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 α, α, β	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 α, β, γ	32 o 1	x, y, z: $0 < x < y < \frac{1}{2}$; $0 < z < \frac{1}{4}$ $\cup$ $\cup$ $x, y, \frac{1}{4}$: $0 < x < y < \frac{1}{2} - x$

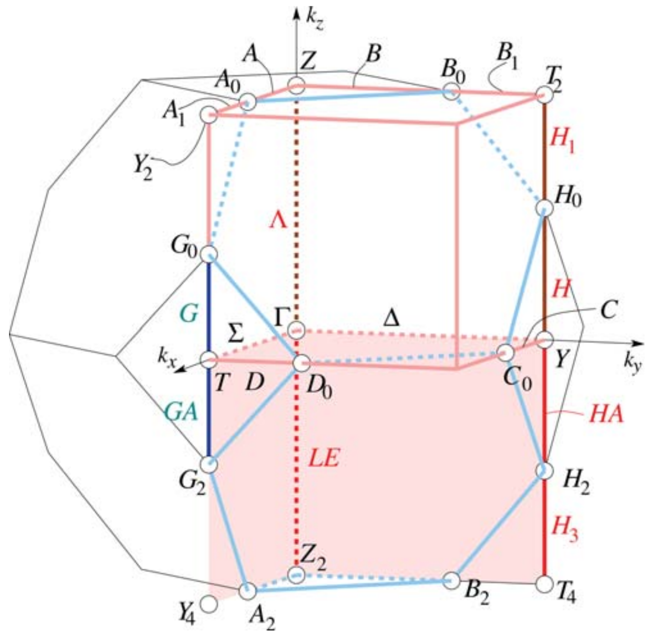


Fig. 1.5.5.5. Brillouin zone with asymmetric unit and representation domain of CDML for arithmetic crystal class *mm*2*F*: $a^{-2} < b^{-2} + c^{-2}$, $b^{-2} < c^{-2} + a^{-2}$ and $c^{-2} < a^{-2} + b^{-2}$. Space groups $Fmm2 - C_{2v}^{18}$ (42), $Fdd2 - C_{2v}^{19}$ (43). Reciprocal-space group (*Imm*2)*, 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
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	$0, 0, z$: $-\frac{1}{2} < z < 0$
$\Gamma \cup \Lambda \cup Z \cup LE$	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	$0, \frac{1}{2}, z$: $-\frac{1}{2} < z \le \frac{1}{2}$
Σ $0, \alpha, \alpha$	*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.*	$x, 0, z$: $0 < x < \frac{1}{2}$; $0 < z \le \frac{1}{2}$
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..*	$0, y, \frac{1}{2}$: $0 < y < b_0$
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 α, β, γ	8 *e* 1	x, y, z: $0 < x, y < \frac{1}{2}$; $0 < z \le \frac{1}{2}$

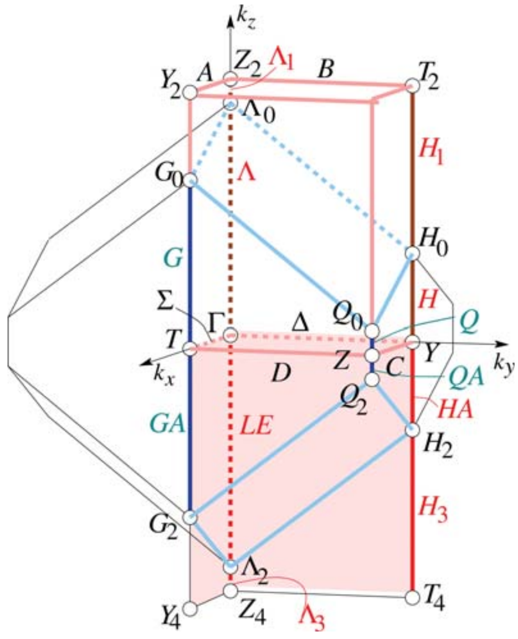


Fig. 1.5.5.6. Brillouin zone with asymmetric unit and representation domain of CDML for arithmetic crystal class *mm*2*F*: $c^{-2} > a^{-2} + b^{-2}$. Space groups $Fmm2 - C_{2v}^{18}$ (42), $Fdd2 - C_{2v}^{19}$ (43). Reciprocal-space group (*Imm*2)*, No. 44: $c^{*2} > a^{*2} + b^{*2}$ (see Table 1.5.5.6). 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 $m\overline{3}mI$ 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 $m\overline{3}mI$ 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 $m\overline{3}mI$ and $m\overline{3}I$: 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 mm*2*F*: $c^{-2} > a^{-2} + b^{-2}$

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: $0 < x, y < \frac{1}{2}$; $0 < z \le \frac{1}{2}$

The figure for arithmetic crystal class $m\overline{3}mI$ is shown in Fig. 1.5.5.1 and the corresponding table is Table 1.5.5.1. The figure for arithmetic crystal class $m\overline{3}I$ 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 mm*2*F*: 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

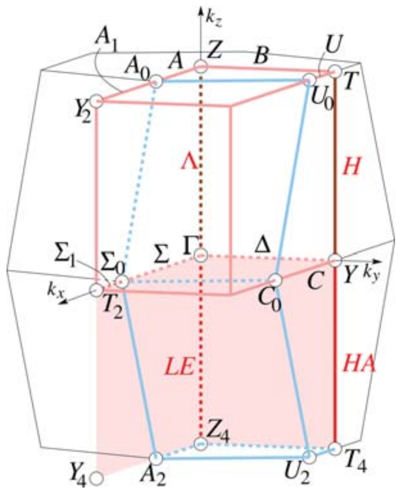


Fig. 1.5.5.7. Brillouin zone with asymmetric unit and representation domain of CDML for arithmetic crystal class $mm2F$: $a^{-2} > b^{-2} + c^{-2}$. Space groups $Fmm2 - C_{2v}^{18}$ (42), $Fdd2 - C_{2v}^{19}$ (43). Reciprocal-space group $(Imm2)^*$, No. 44: $a^{*2} > b^{*2} + c^{*2}$ (see Table 1.5.5.7).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

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; $\overline{x}, x, z$; x, y, x; $x, y, \overline{x}$; x, y, y; $x, \overline{y}, y$. Three of them (x, x, z, $\overline{x}, x, z$ 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) $m..$,

order 2. Consequently, $[\Gamma\ H\ N]$ is $\frac{1}{16}$ of the unit square a^{*2}: $0 < x < y < \frac{1}{2} - x$. In $(Fm\overline{3})^*$, the stabilizer of $x, y, 0$, here $A \cup AA$, is mmm. and $t(\frac{1}{2}, \frac{1}{2}, 0)$, order 16, with the same group $\overline{\mathcal{G}}^{\mathbf{k}} = m..$ of order 2. Therefore, $[\Gamma\ H_2\ H]$ is $\frac{1}{8}$ of the unit square a^{*2} in $(Fm\overline{3})^*$; $0 < y < \frac{1}{2} - x < \frac{1}{2}$.

(4) Arithmetic crystal class $m\overline{3}mI$, line $x, x, 0$: In $(Fm\overline{3}m)^*$ the stabilizer is generated by $m.mm$ and $t(\frac{1}{2}, \frac{1}{2}, 0)$ mod (integer translations), order 16, $\overline{\mathcal{G}}^{\mathbf{k}}$ is $m.2m$ of order 4. The divisor is 4 and thus $0 < x < \frac{1}{4}$. In $(Fm\overline{3})^*$ the stabilizer is generated by $2/m..$ and $t(\frac{1}{2}, \frac{1}{2}, 0)$ mod (integer translations), order 8, and $\overline{\mathcal{G}}^{\mathbf{k}} = m..$, order 2; the divisor is 4 again and $0 < x < \frac{1}{4}$ is restricted to the same range.

In the way just described the *inner* part of the parameter range can be fixed. The *boundaries* of the parameter range must be determined in addition:

(1) Arithmetic crystal classes $m\overline{3}mI$ and $m\overline{3}I$, *i.e.* $(Fm\overline{3}m)^*$ and $(Fm\overline{3})^*$, line x, x, x: The points $0, 0, 0$; $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ (and $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$) are special points; the parameter ranges are open: $0 < x < \frac{1}{4}$, $\frac{1}{4} < x < \frac{1}{2}$.

(2) Arithmetic crystal class $m\overline{3}mI$, plane x, x, z: In $(Fm\overline{3}m)^*$ all corners Γ, N, N_2, H_2 and all edges are special points or lines. Therefore, the parameter ranges are open: x, x, z: $0 < x < \frac{1}{4}, 0 < z < \frac{1}{2}$, where the lines x, x, x: $0 < x < \frac{1}{4}$ and $x, x, \frac{1}{2} - x$: $0 < x < \frac{1}{4}$ are special lines and thus excepted.

(3) Arithmetic crystal classes $m\overline{3}mI$ and $m\overline{3}I$, plane $x, y, 0$: In both reciprocal-space groups, $(Fm\overline{3}m)^*$ and $(Fm\overline{3})^*$, $0 < x$ and $0 < y$ holds. The line $0, y, 0 = \Delta$ is a special line, its $\mathbf{k}$ vectors have little co-groups of higher order than that of the planes $x, y, 0$ and the boundaries of both planes are open. The same holds for the boundary $x, 0, 0 \sim 0, y, 0$ for $(Fm\overline{3})^*$. The $\mathbf{k}$ vectors of the lines $x, x, 0$ and $x, \frac{1}{2} - x, 0$, Σ and G, also have little co-groups of higher order and belong to other Wintgen positions in the representation domain (or asymmetric unit) of $(Fm\overline{3}m)^*$. Therefore, for the arithmetic crystal class $m\overline{3}mI$, the plane $A = x, y, 0$ is open at its boundaries $x, x, 0$ and $x, \frac{1}{2} - x, 0$ in the range $0 < x < \frac{1}{4}$. In the asymmetric unit of $(Fm\overline{3})^*$ the lines $x, x, 0$: $0 < x < \frac{1}{4}$ and $x, \frac{1}{2} - x, 0$: $0 < x < \frac{1}{4}$ belong to the plane, and the boundary of the plane A is here closed. The boundary line $x, \frac{1}{2} - x, 0$: $\frac{1}{4} < x < \frac{1}{2}$ of the plane AA is equivalent to the range $0 < x < \frac{1}{4}$ of the part A and thus does not belong to the asymmetric unit; here the boundary of the plane $A \cup AA$ is open.

1.5.6. Conclusions

International Tables for Crystallography Volume A can serve as a basis for the classification of irreps of space groups by using the concept of reciprocal-space groups. The main features of the crystallographic classification scheme are as follows.

(i) The asymmetric units of the conventional crystallographic unit cells are minimal domains of $\mathbf{k}$ space which are in many cases simpler than the representation domains of the Brillouin zones.

(ii) All $\mathbf{k}$-vector stars giving rise to the same type of irreps belong to the same Wintgen position and *vice versa*. They can be collected in one entry (uni-arm description) and are designated by the same Wintgen letter if flagpoles and wings are admitted.

(iii) The Wyckoff positions of *IT* A, interpreted as Wintgen positions, provide a complete list of the special $\mathbf{k}$ vectors in the Brillouin zone; the site symmetry of *IT* A is the little co-group $\overline{\mathcal{G}}^{\mathbf{k}}$ of $\mathbf{k}$; the multiplicity per primitive unit cell is the number of arms of the star of $\mathbf{k}$. The Wintgen positions with 0, 1, 2, or 3 variable parameters correspond to special $\mathbf{k}$-vector points, $\mathbf{k}$-vector lines, $\mathbf{k}$-vector planes or to the set of all general $\mathbf{k}$ vectors, respectively.

The complete set of types of irreps is obtained by considering the irreps of one $\mathbf{k}$ vector per Wintgen position in the uni-arm description. A complete set of inequivalent irreps of $\mathcal{G}$ is obtained from these irreps by varying the parameters within their ranges.

Data on the independent parameter ranges are essential to make sure that exactly one $\mathbf{k}$ vector per orbit is represented in the representation domain Φ or in the asymmetric unit. Such data are often much easier to calculate for the asymmetric unit of the unit cell than for the representation domain of the Brillouin zone, in particular if a uni-arm description has been chosen, *cf.* Section 1.5.5. Such data can not be found in the cited tables of irreps.

The uni-arm description unmasks those $\mathbf{k}$ vectors which lie on the boundary of the Brillouin zone but belong to a Wintgen position which also contains inner $\mathbf{k}$ vectors, see the example of the lines Λ and F in $(Fm\overline{3}m)^*$ and $(Fm\overline{3})^*$. Such $\mathbf{k}$ vectors can not give rise to little-group representations obtained from projective representations of the little co-group $\overline{\mathcal{G}}^{\mathbf{k}}$.

The consideration of the basic domain Ω in relation to the representation domain Φ is unnecessary. It may even be misleading because special $\mathbf{k}$-vector subspaces of Ω frequently belong to more general types of $\mathbf{k}$ vectors in Φ. Space groups $\mathcal{G}$ with non-holohedral point groups can be referred to their reciprocal-space groups $(\mathcal{G})^*$ directly without reference to the types of irreps of the corresponding holosymmetric space group.

In principle both approaches are equivalent: the *traditional* one by Brillouin zone, basic domain and representation domain and the *crystallographic* one by unit cell and asymmetric unit. Moreover, it is not difficult to relate one approach to the other, see Figs. and Tables 1.5.5.1 to 1.5.5.7. The conclusions show that the crystallographic approach for the description of irreps of space groups has several advantages as compared with the traditional approach. Owing to these advantages, CDML have already accepted the crystallographic approach for triclinic and monoclinic space groups. However, the advantages are not restricted to such low symmetries. In particular, the simple boundary conditions and shapes of the asymmetric units result in simple equations for the boundaries and shapes of volume elements and facilitate numerical calculations, integrations *etc.* If there are special reasons to prefer $\mathbf{k}$ vectors inside or on the boundary of the Brillouin zone to those outside, then the advantages and disadvantages of both approaches have to be compared in order to find the optimal way to solve the problem.

The crystallographic approach may be realized in three different ways:

(1) In the *uni-arm description* one lists each $\mathbf{k}$-vector star exactly once by indicating the parameter field of the representing $\mathbf{k}$ vector. Advantages are the transparency of the presentation and the relatively small effort for the derivation of the list. A disadvantage may be that there are protruding flagpoles or wings. Points of flagpoles or wings are no longer neighbours of inner points (an inner point has a full three-dimensional sphere of neighbours which belong to the asymmetric unit).

(2) In the *compact description* one lists each $\mathbf{k}$ vector exactly once such that each point of the asymmetric unit is either an inner point itself or has inner points as neighbours. Such a description may not be uni-arm for some Wintgen positions, and the determination of the parameter ranges may become less straightforward.

(3) In the *non-unique description* one gives up the condition that each $\mathbf{k}$ vector is listed exactly once. The uni-arm and the compact descriptions are combined but the equivalence relations ($\sim$) are stated explicitly for those $\mathbf{k}$ vectors which occur in more than one entry. Such tables are most informative and not too complicated for practical applications.

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