*International Tables for Crystallography* (2010). Vol. B, Section 1.5.5.1, pp. 182–184.



## 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 $m\overline{3}mI$ (space groups $Im\overline{3}m$ and $Ia\overline{3}d$), reciprocal-space group $(\mathcal{G})^*$ isomorphic to $Fm\overline{3}m$. 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 $m\overline{3}I$ (space groups $Im\overline{3}$ and $Ia\overline{3}$), reciprocal-space group $(\mathcal{G})^*$ isomorphic to $Fm\overline{3}$. 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 $\Gamma$.

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 $\Lambda_0$ is $\lambda_0$ *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.

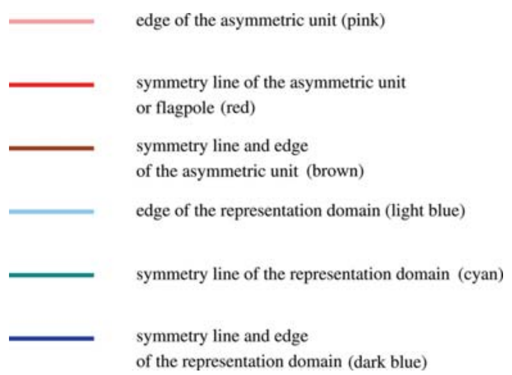
The representatives for the orbits of symmetry points or of symmetry lines, as well as the edges of the representation domain of CDML and of the chosen asymmetric unit are shown in colour.

(*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.

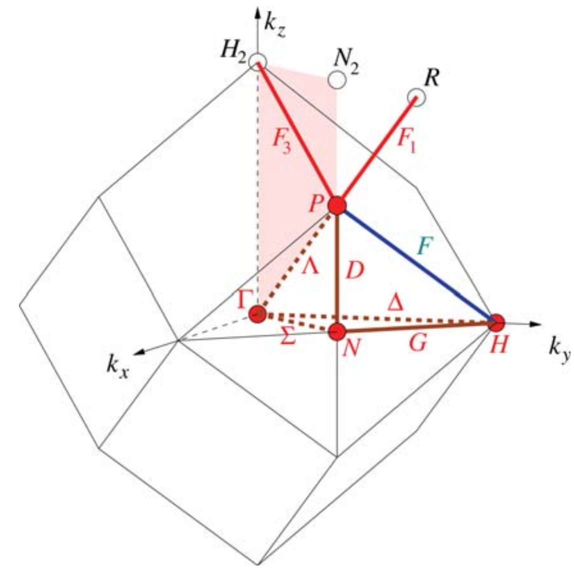



Fig. 1.5.5.1. Brillouin zone with asymmetric unit and representation domain of CDML for arithmetic crystal class $m\bar{3}mI$. Space groups: $Im\bar{3}m - O_h^9$ (229), $Ia\bar{3}d - O_h^{10}$ (230). Reciprocal-space group $(Fm\bar{3}m)^*$, No. 225 (see Table 1.5.5.1). The representation domain of CDML 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 |
|---|---|---|
| $\Gamma$ $\;0, 0, 0$ | 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* $m.mm$ | $\frac{1}{4}, \frac{1}{4}, 0$ |
| $\Delta$ $\;\alpha, -\alpha, \alpha$ | 24 *e* $4m.m$ | $0, y, 0$: $0 < y < \frac{1}{2}$ |
| $\Lambda$ $\;\alpha, \alpha, \alpha$ | *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* $2.mm$ | $\frac{1}{4}, \frac{1}{4}, z$: $0 < z < \frac{1}{4}$ |
| $\Sigma$ $\;0, 0, \alpha$ | 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* $..m$ | $x, \frac{1}{2} - x, z$: $0 < z < x < \frac{1}{4}$ |
| $B \sim B_1 = [P\,N_2\,H_2]$ | | $x, x, z$: $0 < x < \frac{1}{2} - x < z < \frac{1}{2}$ |
| $C$ $\;\alpha, \alpha, \beta$ | *ex* 96 *k* $..m$ | $x, x, z$: $0 < z < x < \frac{1}{4}$ |
| $J$ $\;\alpha, \beta, \alpha$ | *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 $z \neq x, z \neq \frac{1}{2} - x$ |
| $GP$ $\;\alpha, \beta, \gamma$ | 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 '$\sim$' 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 $C$.

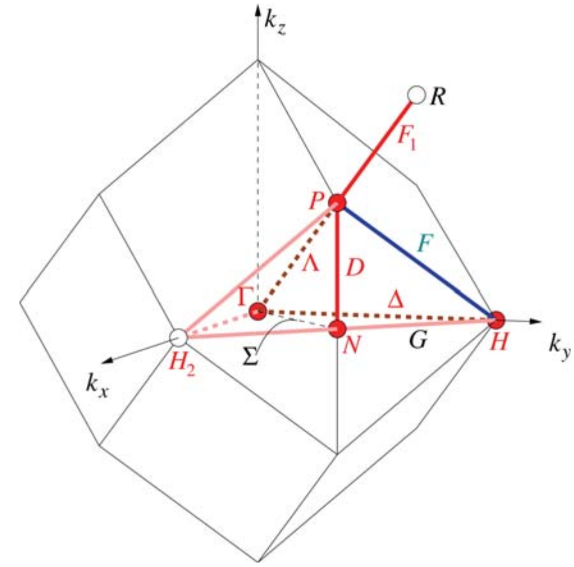



Fig. 1.5.5.2. Brillouin zone with asymmetric unit and representation domain of CDML for arithmetic crystal class $m\bar{3}I$. Space groups $Im\bar{3} - T_h^5$ (204), $Ia\bar{3} - T_h^7$ (206). Reciprocal-space group $(Fm\bar{3})$*, No. 202 (see Table 1.5.5.2). The representation domain of CDML is identical 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* $m..$ | $x, y, 0$: $0 < y < \frac{1}{2} - x < \frac{1}{2}$ $\cup$ <br> $\cup$ $x, \frac{1}{2} - x, 0$: $0 < x < \frac{1}{4}$ |
| $GP$ $\alpha, \beta, \gamma$ | 96 *i* 1 | $x, y, z$: $0 < z \leq x < y < \frac{1}{2} - x$ $\cup$ <br> $\cup$ $x, y, z$: $0 < z < y < x \leq \frac{1}{2} - y$ $\cup$ <br> $\cup$ $x, x, z$: $0 < z < x < \frac{1}{4}$ |