

1. GENERAL RELATIONSHIPS AND TECHNIQUES

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 \mathbf{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 \mathbf{k} vectors in CDML, Tables 3.9 and 3.11 and parameter description of CDML for the set of \mathbf{k} vectors which belong to the label. No ranges for the parameters are listed in CDML.

If two \mathbf{k} vectors belong to the same type of \mathbf{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 \mathbf{k} vectors with the *same* CDML label always belong to the same \mathbf{k} -vector type. \mathbf{k} vectors with *different* CDML labels may either belong to the same or to different types of \mathbf{k} vectors. If such \mathbf{k} vectors belong to the same type, the corresponding Wyckoff-position descriptions are preceded by the letters 'ex'. Frequently, such \mathbf{k} vectors have been transformed (sign ' \sim ' in these tables) to equivalent ones in order to make the \mathbf{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 .

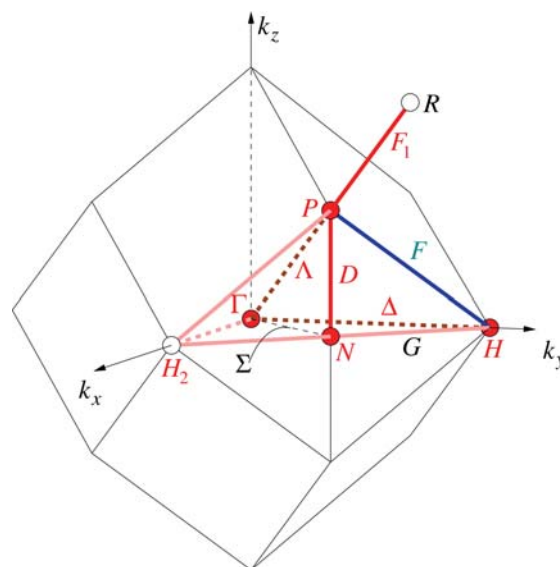


Fig. 1.5.5.2. Brillouin zone with asymmetric unit and representation domain of CDML for arithmetic crystal class $m\bar{3}I$. Space groups $Im\bar{3} - T_h^7$ (204), $Ia\bar{3} - T_h^7$ (206). Reciprocal-space group $(Fm\bar{3})^*$, No. 202 (see Table 1.5.5.2). The representation domain of CDML is identical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

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 $[\Gamma R][P]$ and $[\Gamma N N_2 H_2][\Lambda, F_3]$ 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 \mathbf{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 \mathbf{k}

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

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

\mathbf{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.	$x, \frac{1}{2} - x, x: 0 < x < \frac{1}{4}$
$F \sim F_1 = [PR]$		$x, x, x: \frac{1}{4} < x < \frac{1}{2}$
$\Lambda \cup F_1 \sim [\Gamma R][P]$	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, α	ex 48 h $m..$	$x, x, 0: 0 < x < \frac{1}{4}$
G $\frac{1}{2} - \alpha, -\frac{1}{2} + \alpha, \frac{1}{2}$	ex 48 h $m..$	$x, \frac{1}{2} - x, 0: 0 < x < \frac{1}{4}$
$A = [\Gamma N H]$ $\alpha, -\alpha, \beta$	ex 48 h $m..$	$x, y, 0: 0 < x < y < \frac{1}{2} - x$
$AA = [\Gamma H_2 N]$ $-\alpha, \alpha, \beta$	ex 48 h $m..$	$x, y, 0: 0 < y < x < \frac{1}{2} - y$
$\Sigma \cup G \cup A \cup AA$	48 h $m..$	$x, y, 0: 0 < y < \frac{1}{2} - x < \frac{1}{2} \cup$ $\cup x, \frac{1}{2} - x, 0: 0 < x < \frac{1}{4}$
GP α, β, γ	96 i 1	$x, y, z: 0 < z \leq x < y < \frac{1}{2} - x \cup$ $\cup x, y, z: 0 < z < y < x \leq \frac{1}{2} - y \cup$ $\cup x, x, z: 0 < z < x < \frac{1}{4}$