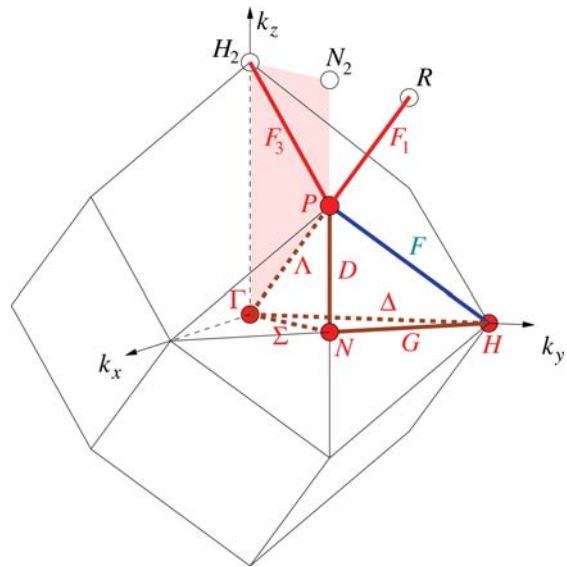


1.5. CLASSIFICATION OF SPACE-GROUP REPRESENTATIONS

(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:

- edge of the asymmetric unit (pink)
- symmetry line of the asymmetric unit or flagpole (red)
- symmetry line and edge of the asymmetric unit (brown)
- edge of the representation domain (light blue)
- symmetry line of the representation domain (cyan)
- symmetry line and edge of the representation domain (dark blue)



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 $m\bar{3}ml$. Space groups: $Im\bar{3}m - O_h^h(229)$, $Ia\bar{3}d - O_h^i(230)$. 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: $F_1 = [PR] \ x, x, x: \frac{1}{4} < x < \frac{1}{2}$. Wing: $B_1 \cup J_1 = [\Gamma P N_2 H_2][F_3] \ x, x, z: 0 < x < \frac{1}{4}, x < z < \frac{1}{2}$ 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 $F \sim F_1 = [PR]$ 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 $m\bar{3}ml$

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 $4\bar{3}m$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$
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 $.3m$	$x, \frac{1}{2} - x, x: 0 < x < \frac{1}{4}$
$F \sim F_1 = [PR]$		x, x, x: $\frac{1}{4} < x < \frac{1}{2}$
$F \sim F_3 = [P H_2]$		$x, x, \frac{1}{2} - x: 0 < x < \frac{1}{4}$
$\Lambda \cup F_1 = [\Gamma R][P]$	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, α	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: $0 < x < z < \frac{1}{2} - x$
$C \cup B_1 \cup J_1 = [\Gamma N N_2 H_2][\Lambda, F_3]$	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: $0 < z < x < y < \frac{1}{2} - x$