

## 1. GENERAL RELATIONSHIPS AND TECHNIQUES

Table 1.5.5.1. The  $\mathbf{k}$ -vector types for the space groups  $Im\bar{3}m$  and  $Ia\bar{3}d$ 

Comparison of the  $\mathbf{k}$ -vector labels and parameters of CDML with the Wyckoff positions of IT A for  $Fm\bar{3}m$ , ( $O_h^5$ ), isomorphic to the reciprocal-space group  $G^*$  of  $m\bar{3}mI$ . The parameter ranges in the last column are chosen such that each star of  $\mathbf{k}$  is represented exactly once. The sign  $\sim$  means symmetrically equivalent. The coordinates  $x, y, z$  of IT A are related to the  $\mathbf{k}$ -vector coefficients of CDML by  $x = 1/2(k_2 + k_3)$ ,  $y = 1/2(k_1 + k_3)$ ,  $z = 1/2(k_1 + k_2)$ .

$\mathbf{k}$ -vector label, CDML	Wyckoff position, IT A	Parameters (see Fig. 1.5.5.1b), IT A
$\Gamma 0, 0, 0$	$4 a m\bar{3}m$	$0, 0, 0$
$H \frac{1}{2}, -\frac{1}{2}, \frac{1}{2}$	$4 b m\bar{3}m$	$\frac{1}{2}, 0, 0$
$P \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$8 c \bar{4}3m$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$
$N 0, 0, \frac{1}{2}$	$24 d m.m.m$	$\frac{1}{4}, \frac{1}{4}, 0$
$\Delta \alpha, -\alpha, \alpha$	$24 e 4m.m$	$x, 0, 0: 0 < x < \frac{1}{2}$
$\Lambda \alpha, \alpha, \alpha$	$32 f .3m$	$x, x, x: 0 < x < \frac{1}{4}$
$F \frac{1}{2} - \alpha, -\frac{1}{2} + 3\alpha, \frac{1}{2} - \alpha$	$32 f .3m$	$\frac{1}{2} - x, x, x: 0 < x < \frac{1}{4}$
$\sim F_1$ (Fig. 1.5.5.1b)	$32 f .3m$	$x, x, x: \frac{1}{4} < x < \frac{1}{2}$
$\sim F_2$ (Fig. 1.5.5.1b)	$32 f .3m$	$x, x, \frac{1}{2} - x: 0 < x < \frac{1}{4}$
$\Lambda \cup F_1 \sim \Gamma H_2 \setminus P$	$32 f .3m$	$x, x, x: 0 < x < \frac{1}{2}$ with $x \neq \frac{1}{4}$
$D \alpha, \alpha, \frac{1}{2} - \alpha$	$48 g 2.m.m$	$\frac{1}{4}, \frac{1}{4}, z: 0 < z < \frac{1}{4}$
$\Sigma 0, 0, \alpha$	$48 h m.m2$	$x, x, 0: 0 < x < \frac{1}{4}$
$G \frac{1}{2} - \alpha, -\frac{1}{2} + \alpha, \frac{1}{2}$	$48 i m.m2$	$\frac{1}{2} - x, x, 0: 0 < x < \frac{1}{4}$
$A \alpha, -\alpha, \beta$	$96 j m..$	$x, y, 0: 0 < y < x < \frac{1}{2} - y$
$B \alpha + \beta, -\alpha + \beta, \frac{1}{2} - \beta$	$96 k ..m$	$\frac{1}{4} + x, \frac{1}{4} - x, z: 0 < z < \frac{1}{4} - x < \frac{1}{4}$
$\sim PH_1 N_1$ (Fig. 1.5.5.1b)	$96 k ..m$	$x, x, z: 0 < x < \frac{1}{2} - x < z < \frac{1}{2}$
$C \alpha, \alpha, \beta$	$96 k ..m$	$x, x, z: 0 < z < x < \frac{1}{4}$
$J \alpha, \beta, \alpha$	$96 k ..m$	$x, y, y: 0 < y < x < \frac{1}{2} - y$
$\sim \Gamma PH_1$ (Fig. 1.5.5.1b)	$96 k ..m$	$x, x, z: 0 < x < z < \frac{1}{2} - x$
$C \cup B \cup J \sim \Gamma NN_1 H_1$	$96 k ..m$	$x, x, z: 0 < x < \frac{1}{4}, 0 < z < \frac{1}{2}$ with $z \neq x, z \neq \frac{1}{2} - x$
$GP \alpha, \beta, \gamma$	$192 l 1$	$x, y, z: 0 < z < y < x < \frac{1}{2} - y$

For non-holosymmetric space groups the representation domain  $\Phi$  is a multiple of the basic domain  $\Omega$ . CDML introduced new letters for stars of  $\mathbf{k}$  vectors in those parts of  $\Phi$  which do not belong to  $\Omega$ . If one can make a new  $\mathbf{k}$  vector uni-arm to some  $\mathbf{k}$  vector of the basic domain  $\Omega$  by an appropriate choice of  $\Phi$  and  $\Omega$ , one can extend the parameter range of this  $\mathbf{k}$  vector of  $\Omega$  to  $\Phi$  instead of introducing new letters. It turns out that indeed most of these new letters are unnecessary. This restricts the introduction of new types of  $\mathbf{k}$  vectors to the few cases where it is indispensable. Extension of the parameter range for  $\mathbf{k}$  means that the corresponding representations can also be obtained by parameter variation. Such representations can be considered to belong to the same type. In this way a large number of superfluous  $\mathbf{k}$ -vector names, which pretend a greater variety of types of irreps than really exists, can be avoided (Boyle, 1986). For examples see Section 1.5.5.1.

## 1.5.5. Examples and conclusions

## 1.5.5.1. Examples

In this section, four examples are considered in each of which the crystallographic classification scheme for the irreps is compared with the traditional one:<sup>†</sup>

<sup>†</sup> Corresponding tables and figures for all space groups are available at [http://www.cryst.ehu.es/cryst/get\\_kvec.html](http://www.cryst.ehu.es/cryst/get_kvec.html).

(1)  $\mathbf{k}$ -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 isomorphic to  $Fm\bar{3}m$ ;  $\Phi = \Omega$ ; see Table 1.5.5.1 and Fig. 1.5.5.1;

(2)  $\mathbf{k}$ -vector types of the arithmetic crystal class  $m\bar{3}I$  ( $Im\bar{3}$  and  $Ia\bar{3}$ ), reciprocal-space group isomorphic to  $Fm\bar{3}$ ,  $\Phi > \Omega$ ; see Table 1.5.5.2 and Fig. 1.5.5.2;

(3)  $\mathbf{k}$ -vector types of the arithmetic crystal class  $4/mmmI$  ( $I4/mmm, I4/mcm, I4_1/and$  and  $I4_1/acd$ ), reciprocal-space group isomorphic to  $I4/mmm$ . Here  $\Phi = \Omega$  changes for different ratios of the lattice constants  $a$  and  $c$ ; see Table 1.5.5.3 and Fig. 1.5.5.3;

(4)  $\mathbf{k}$ -vector types of the arithmetic crystal class  $mm2F$  ( $Fmm2$  and  $Fdd2$ ), reciprocal-space group isomorphic to  $Imm2$ . Here  $\Phi > \Omega$  changes for different ratios of the lattice constants  $a, b$  and  $c$ ; see Table 1.5.5.4 and Fig. 1.5.5.4.

The asymmetric units of IT A are displayed in Figs. 1.5.5.1 to 1.5.5.4 by dashed lines. In Tables 1.5.5.1 to 1.5.5.4, the  $\mathbf{k}$ -vector types of CDML are compared with the Wintgen (Wyckoff) positions of IT A. The parameter ranges are chosen such that each star of  $\mathbf{k}$  is represented exactly once. Sets of symmetry points, lines or planes of CDML which belong to the same Wintgen position are separated by horizontal lines in Tables 1.5.5.1 to 1.5.5.3. The uni-arm description is listed in the last entry of each Wintgen position in Tables 1.5.5.1 and 1.5.5.2. In Table 1.5.5.4, so many  $\mathbf{k}$ -vector types of CDML belong to each Wintgen position that the latter are used as headings under which the CDML types are listed.