

1. GENERAL RELATIONSHIPS AND TECHNIQUES

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

Comparison of the **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  $\mathcal{G}^*$  of  $m\bar{3}mI$ . The parameter ranges in the last column are chosen such that each star of **k** is represented exactly once. The sign  $\sim$  means symmetrically equivalent. The coordinates  $x, y, z$  of *IT A* are related to the **k**-vector coefficients of CDML by  $x = 1/2(k_2 + k_3)$ ,  $y = 1/2(k_1 + k_3)$ ,  $z = 1/2(k_1 + k_2)$ .

<b>k</b> -vector label, CDML	Wyckoff position, <i>IT A</i>	Parameters (see Fig. 1.5.5.1b), <i>IT A</i>
$\Gamma$ 0, 0, 0	4 <i>a</i> $m\bar{3}m$	0, 0, 0
$H$ $\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}$	4 <i>b</i> $m\bar{3}m$	$\frac{1}{2}, 0, 0$
$P$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	8 <i>c</i> $\bar{4}3m$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$
$N$ 0, 0, $\frac{1}{2}$	24 <i>d</i> $m.mm$	$\frac{1}{4}, \frac{1}{4}, 0$
$\Delta$ $\alpha, -\alpha, \alpha$	24 <i>e</i> $4m.m$	$x, 0, 0: 0 < x < \frac{1}{2}$
$\Lambda$ $\alpha, \alpha, \alpha$ $F$ $\frac{1}{2} - \alpha, -\frac{1}{2} + 3\alpha, \frac{1}{2} - \alpha$ $\sim F_1$ (Fig. 1.5.5.1b) $\sim F_2$ (Fig. 1.5.5.1b) $\Lambda \cup F_1 \sim \Gamma H_2 \setminus P$	32 <i>f</i> $.3m$ 32 <i>f</i> $.3m$ 32 <i>f</i> $.3m$ 32 <i>f</i> $.3m$ 32 <i>f</i> $.3m$	$x, x, x: 0 < x < \frac{1}{4}$ $\frac{1}{2} - x, x, x: 0 < x < \frac{1}{4}$ $x, x, x: \frac{1}{4} < x < \frac{1}{2}$ $x, x, \frac{1}{2} - x: 0 < x < \frac{1}{4}$ $x, x, x: 0 < x < \frac{1}{2}$ with $x \neq \frac{1}{4}$
$D$ $\alpha, \alpha, \frac{1}{2} - \alpha$	48 <i>g</i> $2.mm$	$\frac{1}{4}, \frac{1}{4}, z: 0 < z < \frac{1}{4}$
$\Sigma$ 0, 0, $\alpha$	48 <i>h</i> $m.m2$	$x, x, 0: 0 < x < \frac{1}{4}$
$G$ $\frac{1}{2} - \alpha, -\frac{1}{2} + \alpha, \frac{1}{2}$	48 <i>i</i> $m.m2$	$\frac{1}{2} - x, x, 0: 0 < x < \frac{1}{4}$
$A$ $\alpha, -\alpha, \beta$	96 <i>j</i> $m..$	$x, y, 0: 0 < y < x < \frac{1}{2} - y$
$B$ $\alpha + \beta, -\alpha + \beta, \frac{1}{2} - \beta$ $\sim PH_1N_1$ (Fig. 1.5.5.1b) $C$ $\alpha, \alpha, \beta$ $J$ $\alpha, \beta, \alpha$ $\sim \Gamma PH_1$ (Fig. 1.5.5.1b) $C \cup B \cup J \sim \Gamma NN_1H_1$	96 <i>k</i> $.m$ 96 <i>k</i> $.m$ 96 <i>k</i> $.m$ 96 <i>k</i> $.m$ 96 <i>k</i> $.m$ 96 <i>k</i> $.m$	$\frac{1}{4} + x, \frac{1}{4} - x, z: 0 < z < \frac{1}{4} - x < \frac{1}{4}$ $x, x, z: 0 < x < \frac{1}{2} - x < z < \frac{1}{2}$ $x, x, z: 0 < z < x < \frac{1}{4}$ $x, y, y: 0 < y < x < \frac{1}{2} - y$ $x, x, z: 0 < x < z < \frac{1}{2} - x$ $x, x, z: 0 < x < \frac{1}{4}, 0 < z < \frac{1}{2}$ with $z \neq x, z \neq \frac{1}{2} - x$ .
$GP$ $\alpha, \beta, \gamma$	192 <i>l</i> 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 **k** vectors in those parts of  $\Phi$  which do not belong to  $\Omega$ . If one can make a new **k** vector uni-arm to some **k** vector of the basic domain  $\Omega$  by an appropriate choice of  $\Phi$  and  $\Omega$ , one can extend the parameter range of this **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 **k** vectors to the few cases where it is indispensable. Extension of the parameter range for **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 **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:†

† 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) **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) **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) **k**-vector types of the arithmetic crystal class  $4/mmmI$  ( $I4/mmm, I4/mcm, I4_1/amd$  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) **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 **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 **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 **k**-vector types of CDML belong to each Wintgen position that the latter are used as headings under which the CDML types are listed.

## 1.5. CLASSIFICATION OF SPACE-GROUP REPRESENTATIONS

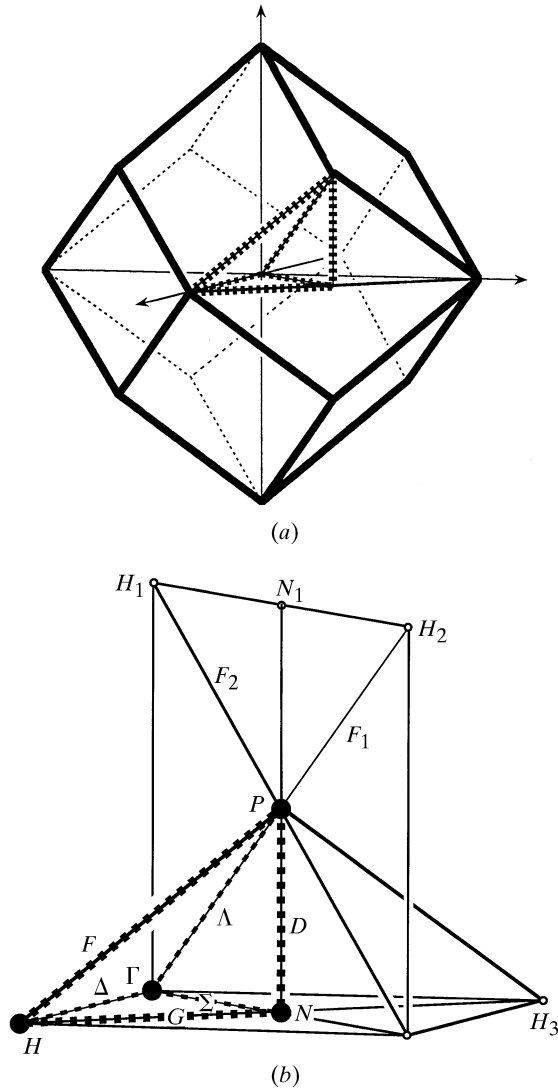


Fig. 1.5.5.1. Symmorphic space group  $Fm\bar{3}m$  (isomorphic to the reciprocal space group  $\mathcal{G}^*$  of  $m\bar{3}m$ ). (a) The asymmetric unit (thick dashed edges) imbedded in the Brillouin zone, which is a cubic rhombododecahedron. (b) The asymmetric unit  $\Gamma HNP$ , IT A, p. 678. The representation domain  $\Gamma NH_3P$  of CDML is obtained by reflecting  $\Gamma HNP$  through the plane of  $\Gamma NP$ . Coordinates of the points:  $\Gamma = 0, 0, 0$ ;  $N = \frac{1}{4}, \frac{1}{4}, 0 \sim N_1 = \frac{1}{4}, \frac{1}{4}, \frac{1}{2}$ ;  $H = \frac{1}{2}, 0, 0 \sim H_1 = 0, 0, \frac{1}{2} \sim H_2 = \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \sim H_3 = 0, \frac{1}{2}, 0$ ;  $P = \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ ; the sign  $\sim$  means symmetrically equivalent. Lines:  $\Lambda = \Gamma P = x, x, x$ ;  $F = HP = \frac{1}{2} - x, x, x \sim F_1 = PH_2 = x, x, x \sim F_2 = PH_1 = x, x, \frac{1}{2} - x$ ;  $\Delta = \Gamma H = x, 0, 0$ ;  $\Sigma = \Gamma N = x, x, 0$ ;  $D = NP = \frac{1}{4}, \frac{1}{4}, z$ ;  $G = NH = x, \frac{1}{2} - x, 0$ . Planes:  $A = \Gamma HN = x, y, 0$ ;  $B = HNP = x, \frac{1}{2} - x, z \sim PN_1H_1 = x, x, z$ ;  $C = \Gamma NP = x, x, z$ ;  $J = \Gamma HP = x, y, y \sim \Gamma PH_1 = x, x, z$ . Large black circles: corners of the asymmetric unit (special points); small open circles: other special points; dashed lines: edges of the asymmetric unit (special lines). For the parameter ranges see Table 1.5.5.1.

### 1.5.5.2. Results

(1) The higher the symmetry of the point group  $\bar{\mathcal{G}}$  of  $\mathcal{G}$ , the more one is restricted in the choice of the boundaries of the minimal domain. 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. However, even for holosymmetric space groups of highest symmetry, the description by Brillouin zone and representation domain is not as concise as possible, cf. CDML.

Examples:

(a) In  $m\bar{3}m$  and  $m\bar{3}I$  there are the  $\Lambda$  and  $F$  lines of  $\mathbf{k}$  vectors  $\mathbf{k}_1(\alpha, \alpha, \alpha)$  and  $\mathbf{k}_2(\frac{1}{2} - \alpha, -\frac{1}{2} + 3\alpha, \frac{1}{2} - \alpha)$  in CDML, see Tables 1.5.5.1 and 1.5.5.2, Figs. 1.5.5.1 and 1.5.5.2. Do they belong to the same Wintgen position, i.e. do their irreps belong to the same type? There is a twofold rotation  $2x, \frac{1}{4}, \frac{1}{4}$  which maps  $\mathbf{k}_2$  onto  $\mathbf{k}'_2 = (\frac{1}{2} - \alpha, \frac{1}{2} - \alpha, \frac{1}{2} - \alpha \in F_1)$  (the rotation  $2$  is described in the primitive basis of CDML by  $k'_1 = k_3, k'_2 = -k_1 - k_2 - k_3 + 1, k'_3 = k_1$ ). The  $\mathbf{k}$  vectors  $\mathbf{k}_1$  and  $\mathbf{k}'_2$  are uni-arm and form the line  $\Gamma H_2 \setminus P = \Lambda \cup F_1 \sim \Lambda \cup F$  which protrudes from the body of the asymmetric unit like a flagpole. This proves that  $\mathbf{k}_1$  and  $\mathbf{k}_2$  belong to the same Wintgen position, which is  $32f.3m\ x, x, x$ .

Owing to the shape of the asymmetric unit of  $IT A$  (which is similar here to that of the representation domain in CDML), the line  $x, x, x$  is kinked into the parts  $\Lambda$  and  $F$ . One may choose even between  $F_1$  (uni-arm to  $\Lambda$ ) or  $F_2$  (completing the plane  $C = \Gamma NP$ ). The latter transformation is performed by applying the symmetry operation  $3^- x, x, x$  for  $F \rightarrow F_2$ .

Remark. The uni-arm description unmasks those  $\mathbf{k}$  vectors (e.g. those of line  $F$ ) which lie on the boundary of the Brillouin zone but belong to a Wintgen position which also contains inner  $\mathbf{k}$  vectors (line  $\Lambda$ ). Such  $\mathbf{k}$  vectors cannot give rise to little-group representations obtained from projective representations of the little co-group  $\bar{\mathcal{G}}^k$ .

(b) In Table 1.5.5.1 for  $m\bar{3}m$ , see also Fig. 1.5.5.1, the  $\mathbf{k}$ -vector planes  $B = HNP$ ,  $C = \Gamma NP$  and  $J = \Gamma HP$  of CDML belong to the same Wintgen position  $96k..m$ . In the asymmetric unit of  $IT A$  (as in the representation domain of CDML) the plane  $x, x, z$  is kinked into parts belonging to different arms of the star of  $\mathbf{k}$ . Transforming, e.g.,  $B$  and  $J$  to the plane of  $C$  by  $2\frac{1}{4}, y, \frac{1}{4}(B \rightarrow PN_1H_1)$  and  $3^- x, x, x (J \rightarrow \Gamma PH_1)$ , one obtains a complete plane ( $\Gamma NN_1H_1$  for  $C, B$  and  $J$ ) as a uni-arm description of the Wintgen position  $96k..m$ . This plane protrudes from the body of the asymmetric unit like a wing.

Remark. One should avoid the term *equivalent* for the relation between  $\Lambda$  and  $F$  or between  $B, C$  and  $J$  as it is used by Stokes *et al.* (1993). BC, p. 95 give the definition: 'Two  $\mathbf{k}$  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 also express this by saying: 'Two  $\mathbf{k}$  vectors are equivalent if they differ by a vector  $\mathbf{K}$  of the (reciprocal) lattice.' We prefer to extend this equivalence by saying: 'Two  $\mathbf{k}$  vectors  $\mathbf{k}_1$  and  $\mathbf{k}_2$  are equivalent if and only if they belong to the same orbit of  $\mathbf{k}$ ', i.e. if there is a matrix part  $\mathbf{W}$  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). Alternatively, this can be expressed as: 'Two  $\mathbf{k}$  vectors are equivalent if and only if they belong to the same or to translationally equivalent stars of  $\mathbf{k}$ .' The  $\mathbf{k}$  vectors of  $\Lambda$  and  $F$  or of  $B, C$  and  $J$  are not even equivalent under this broader definition, see Davies & Dirl (1987). If the representatives of the  $\mathbf{k}$ -vector stars are chosen uni-arm, as in the examples, their non-equivalence is evident.

(2) In general two trends can be observed:

(a) The lower the symmetry of the crystal system, the more irreps of CDML, recognized by different letters, belong to the same Wintgen position. This trend is due to the splitting of lines and planes into pieces because of the more and more complicated shape of the Brillouin zone. Faces and lines on the surface of the Brillouin zone may appear or disappear depending on the lattice parameters, causing different descriptions of Wintgen positions. This does not happen in unit cells or their asymmetric units; see Sections 1.5.4.1 and 1.5.4.2.

Examples:

(i) The boundary conditions (parameter ranges) for the special lines and planes of the asymmetric unit and for general  $\mathbf{k}$  vectors of

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Table 1.5.5.2. The  $\mathbf{k}$ -vector types for the space groups  $Im\bar{3}$  and  $Ia\bar{3}$

Comparison of the  $\mathbf{k}$ -vector labels and parameters of CDML with the Wyckoff positions of  $IT A$  for  $Fm\bar{3}$  ( $T_h^3$ ), isomorphic to the reciprocal-space group  $\mathcal{G}^*$  of  $m\bar{3}I$ . The parameter ranges in  $Fm\bar{3}$  are obtained by extending those of  $Fm\bar{3}m$  such that each star of  $\mathbf{k}$  is represented exactly once. The  $\mathbf{k}$ -vector types of  $(Fm\bar{3}m)^*$ , see Table 1.5.5.1, are also listed. The sign  $\sim$  means symmetrically equivalent. Lines in parentheses are not special lines but belong to special planes. As in Table 1.5.5.1, the coordinates  $x, y, z$  of  $IT A$  are related to the  $\mathbf{k}$ -vector coefficients of CDML by  $x = 1/2(k_2 + k_3)$ ,  $y = 1/2(k_1 + k_3)$ ,  $z = 1/2(k_1 + k_2)$ .

k-vector label, CDML		Wyckoff position, $IT A$	Parameters (see Fig. 1.5.5.2b), $IT A$
$(Fm\bar{3}m)^*$	$(Fm\bar{3})^*$	$Fm\bar{3}$	
$\Gamma$	$\Gamma$	4 a $m\bar{3}$ .	0, 0, 0
$H$	$H$	4 b $m\bar{3}$ .	$\frac{1}{2}, 0, 0$
$P$	$P$	8 c 23.	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$
$N$	$N$	24 d 2/m..	$\frac{1}{4}, \frac{1}{4}, 0$
$\Delta$	$\Delta$	24 e $mm2$ ..	$x, 0, 0: 0 < x < \frac{1}{2}$
$\Lambda$	$\Lambda$	32 f .3.	$x, x, x: 0 < x < \frac{1}{4}$
$F$	$F$	32 f .3.	$\frac{1}{2} - x, x, x: 0 < x < \frac{1}{4}$
$\sim F_1$	$\sim F_1$	32 f .3.	$x, x, x: \frac{1}{4} < x < \frac{1}{2}$
$\Lambda \cup F_1 \sim \Gamma H_2 \setminus P$	$\Lambda \cup F_1 \sim \Gamma H_2 \setminus P$	32 f .3.	$x, x, x: 0 < x < \frac{1}{2}$ with $x \neq \frac{1}{4}$
$D$	$D$	48 g 2..	$\frac{1}{4}, \frac{1}{4}, z: 0 < z < \frac{1}{4}$
$\Sigma$	$\Sigma$	48 h m..	$x, y, 0: 0 < x = y < \frac{1}{4}$
$G$	$G$	48 h m..	$x, y, 0: 0 < y = \frac{1}{2} - x < \frac{1}{4}$
$A$	$A$	48 h m..	$x, y, 0: 0 < y < x < \frac{1}{2} - y$
	$AA -\alpha, \alpha, \beta$	48 h m..	$x, y, 0: 0 < \frac{1}{2} - x < y < x$
	$A \cup AA \cup \Sigma \cup G$	48 h m..	$x, y, 0: 0 < y < x < \frac{1}{2} \cup$ $\cup 0 < y = x < \frac{1}{4}$
$C$	$\subset GP$	96 i 1	$x, y, z: 0 < z < x = y < \frac{1}{4}$
$B$	$\subset GP$	96 i 1	$x, y, z: 0 < z < y = \frac{1}{2} - x < \frac{1}{4}$
$J$	$\subset GP$	96 i 1	$x, y, z: 0 < z = y < x < \frac{1}{2} - y$
$GP$	$\subset GP$	96 i 1	$x, y, z: 0 < z < y < x < \frac{1}{2} - y$
	$\subset GP$	96 i 1	$x, y, z: 0 < z < \frac{1}{2} - x < y < x$
	$GP$	96 i 1	$x, y, z: 0 < z \leq y \leq x \leq \frac{1}{2} - y \cup$ $\cup x, y, z: 0 < z < \frac{1}{2} - x < y < x$

the reciprocal-space group  $(F4/mmm)^*$  (setting  $I4/mmm$ ) are listed in Table 1.5.5.3. The main condition of the representation domain is that of the boundary plane  $x, y, z = \{1 + (c/a)^2[1 - 2(x + y)]\}/4$ , which for  $c/a < 1$  forms the triangle  $Z_0Z_1P$  (Figs. 1.5.5.3a,b) but for  $c/a > 1$  forms the pentagon  $S_1RPGS$  (Figs. 1.5.5.3c,d). The inner points of these boundary planes 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 for the asymmetric unit (for this the boundary condition is simply  $x, y, \frac{1}{4}$ ).

(ii) In the reciprocal-space group  $(Im\bar{3}m)^*$ , see Figs. 1.5.5.4(a) to (c), the lines  $\Lambda$  and  $Q$  belong to Wintgen position  $2 a mm2$ ;  $G$  and  $H$  belong to  $2 b mm2$ ;  $\Delta$  and  $R, \Sigma$  and  $U, A$  and  $C$ , and  $B$  and  $D$  belong to the general position  $GP$ . The decisive boundary plane is  $x/a^2 + y/b^2 + z/c^2 = d^2/4$ , where  $d^2 = 1/a^2 + 1/b^2 + 1/c^2$ , or  $xa^{*2} + yb^{*2} + zc^{*2} = d^{*2}/4$ , where  $d^{*2} = a^{*2} + b^{*2} + c^{*2}$ . There is no relation of the lattice constants for which all the above-mentioned lines are realized on the surface of the representation domain simultaneously, either two or three of them do not appear and the length of the others depends on the boundary plane; see Table 1.5.5.4 and Figs. 1.5.5.4(a) to (c). Again, the boundary conditions for the asymmetric unit are independent of the lattice parameters, all lines mentioned above are present and their parameters run from 0 to  $\frac{1}{2}$ .

(b) The more symmetry a space group has lost compared to its holosymmetric space group, the more letters of irreps are introduced, cf. CDML. In most cases these additional labels can be easily avoided by extension of the parameter range in the  $\mathbf{k}$ -vector space of the holosymmetric group.

*Example.* Extension of the plane  $A = \Gamma NH$ , Wintgen position 96 j m.. of  $(Fm\bar{3}m)^*$ , to  $A \cup AA = \Gamma_1 NH$  in the reciprocal-space group  $(Fm\bar{3})^*$  of the arithmetic crystal class  $m\bar{3}I$ , cf. Tables 1.5.5.1 and 1.5.5.2 and Fig. 1.5.5.2. Both planes,  $A$  and  $AA$ , belong to Wintgen position 48 h m.. of  $(Fm\bar{3})^*$ .

In addition, in the transition from a holosymmetric space group  $\mathcal{H}$  to a non-holosymmetric space group  $\mathcal{G}$ , the order of the little co-group  $\mathcal{H}^{\mathbf{k}}$  of a special  $\mathbf{k}$  vector of  $\mathcal{H}^*$  may be reduced in  $\mathcal{G}^{\mathbf{k}}$ . Such a  $\mathbf{k}$  vector may then be incorporated into a more general Wintgen position of  $\mathcal{G}^{\mathbf{k}}$  and described by an extension of the parameter range.

*Example.* Plane  $\Gamma H\Gamma_1 = x, y, 0$ : In  $(Fm\bar{3}m)^*$ , see Fig. 1.5.5.1, all points  $(\Gamma, H, N)$  and lines  $(\Delta, \Sigma, G)$  of the boundary of the asymmetric unit are special. In  $(Fm\bar{3})^*$ , see Fig. 1.5.5.2, the lines  $\Delta$  and  $H\Gamma_1 \sim \Delta$  ( $\sim$  means equivalent) are special but  $\Sigma, G$  and  $N\Gamma_1 \sim N\Gamma = \Sigma$  belong to the plane  $(A \cup AA)$ . The free parameter range on the line  $\Gamma\Gamma_1$  is  $\frac{1}{2}$  of the full parameter range of  $\Gamma\Gamma_1$ , see Section 1.5.5.3. Therefore, the parameter ranges of  $(A \cup AA \cup G \cup \Sigma)$  in  $x, y, 0$  can be taken as:  $0 < y < x < \frac{1}{2}$  for  $A \cup AA \cup G$  and (for  $\Sigma$ )  $0 < y = x < \frac{1}{4}$ .

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Is it easy to recognize those letters of CDML which belong to the *same* Wintgen position? In  $(I4/mmm)^*$ , the lines  $\Lambda$  and  $V$  ( $V$  exists for  $c/a < 1$  only) are parallel, as are  $\Sigma$  and  $F$ , but the lines  $Y$  and  $U$  are not ( $F$  and  $U$  exist for  $c/a > 1$  only). The planes  $C = x, y, 0$  and  $D = x, y, \frac{1}{2}$  ( $D$  for  $c/a > 1$  only) are parallel but the planes  $A = 0, y, z$  and  $E = x, \frac{1}{2}, z$  are not. Nevertheless, each of these pairs belongs to one Wintgen position, *i.e.* describes one type of  $\mathbf{k}$  vector.

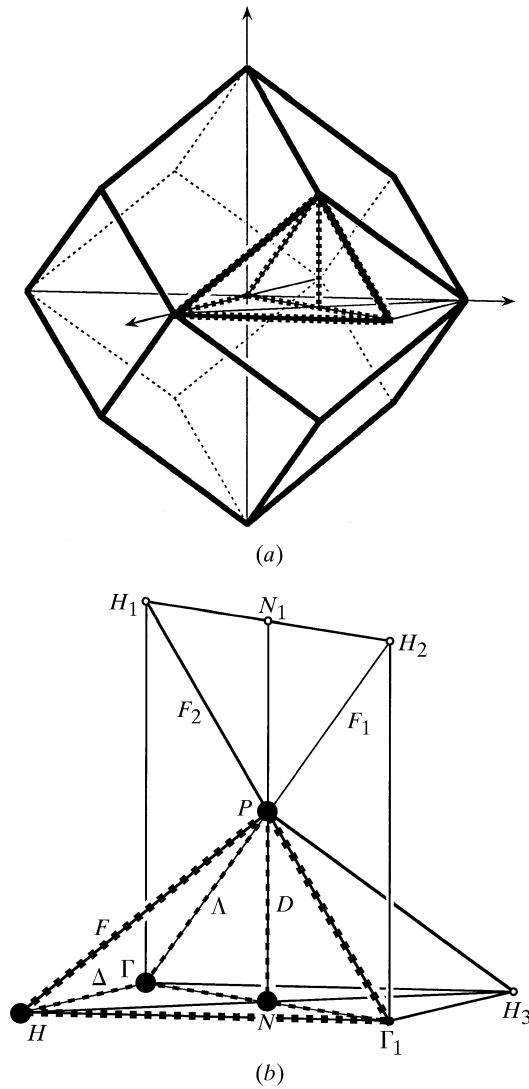


Fig. 1.5.5.2. Symmorphic space group  $F\bar{3}m$  (isomorphic to the reciprocal-space group  $\mathcal{G}^*$  of  $m\bar{3}I$ ). (a) The asymmetric unit (thick dashed edges) half imbedded in and half protruding from the Brillouin zone, which is a cubic rhombododecahedron (as in Fig. 1.5.5.1). (b) The asymmetric unit  $\Gamma H\Gamma_1 P$ , IT A, p. 610. The representation domain of CDML is  $\Gamma H H_3 P$ . Both bodies have  $\Gamma H N P$  in common;  $H\Gamma_1 N P$  is mapped onto  $\Gamma N H_3 P$  by a twofold rotation around  $N P$ . The representation domain as the asymmetric unit would be the better choice because it is congruent to the asymmetric unit of IT A and is fully imbedded in the Brillouin zone. Coordinates of the points:  $\Gamma = 0, 0, 0 \sim \Gamma_1 = \frac{1}{2}, \frac{1}{2}, 0$ ;  $P = \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ ;  $H = \frac{1}{2}, 0, 0 \sim H_1 = 0, 0, \frac{1}{2} \sim H_2 = \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \sim H_3 = 0, \frac{1}{2}, 0$ ;  $N = \frac{1}{4}, \frac{1}{4}, 0 \sim N_1 = \frac{1}{4}, \frac{1}{4}, \frac{1}{2}$ ; the sign  $\sim$  means symmetrically equivalent. Lines:  $\Lambda = \Gamma P = x, x, x \sim P\Gamma_1 = x, x, \frac{1}{2} - x$ ;  $F = HP = \frac{1}{2} - x, x, x \sim F_1 = PH_2 = x, x, x \sim F_2 = PH_1 = x, x, \frac{1}{2} - x$ ;  $\Delta = \Gamma H = x, 0, 0 \sim H\Gamma_1 = \frac{1}{2}, y, 0$ ;  $D = PN = \frac{1}{4}, \frac{1}{4}, z$ . ( $G = NH = x, \frac{1}{2} - x, 0$  and  $\Sigma = GN = x, x, 0 \sim N\Gamma_1 = x, x, 0$  are not special lines.) Planes:  $A = \Gamma H N = x, y, 0$ ;  $AA = \Gamma_1 N H = x, y, 0$ ;  $B = H N P = x, \frac{1}{2} - x, z \sim P N H_1 = x, x, z$ ;  $C = \Gamma N P = x, x, z$ ;  $J = \Gamma H P = x, y, y \sim \Gamma H P_1 = x, x, z$ . (The boundary planes  $B, C$  and  $J$  are parts of the general position  $GP$ .) Large black circles: special points of the asymmetric unit; small black circle: special point  $\Gamma_1 \sim \Gamma$ ; small open circles: other special points; dashed lines: edges and special line  $D$  of the asymmetric unit. The edge  $\Gamma\Gamma_1$  is not a special line but is part of the boundary plane  $A \cup AA$ . For the parameter ranges see Table 1.5.5.2.

### 1.5.5.3. Parameter ranges

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  $\mathbf{k}$  as the parameter space (point, line, plane or space) of a Wintgen position. For the check, one determines that part of the field of  $\mathbf{k}$  which is inside the unit cell. The order of the little co-group  $\bar{\mathcal{G}}^k$  ( $\bar{\mathcal{G}}^k$  represents those operations which leave the field of  $\mathbf{k}$  fixed pointwise) is divided by the order of the stabilizer [which is the set of all symmetry operations (*modulo* integer translations) that leave the field *invariant as a whole*]. The result gives the independent fraction of the above-determined 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. The parameter ranges of the different arms are not necessarily equal; see the second of the following examples.

Examples:

(1) Line  $\Lambda \cup F_1$ : In  $(Fm\bar{3}m)^*$  the line  $x, x, x$  has stabilizer  $\bar{3}m$  and little co-group  $\bar{\mathcal{G}}^k = 3m$ . Therefore, the divisor is 2 and  $x$  runs from 0 to  $\frac{1}{2}$  in  $0 < x < 1$ .

(2) Plane  $B \cup C \cup J$ : In  $(Fm\bar{3}m)^*$ , the stabilizer of  $x, x, z$  is generated by  $m.mm$  and the centring translation  $t(\frac{1}{2}, \frac{1}{2}, 0)$  modulo integer translations ( $\text{mod } \mathbf{T}_{\text{int}}$ ). They generate a group of order 16;  $\bar{\mathcal{G}}^k$  is  $..m$  of order 2. The fraction of the plane is  $\frac{2}{16} = \frac{1}{8}$  of the area  $2^{1/2} a^2$ , as expressed by the parameter ranges  $0 < x < \frac{1}{4}, 0 < z < \frac{1}{2}$ . There are six arms of the star of  $x, x, z$ :  $x, x, z; \bar{x}, x, z; x, y, x; x, y, \bar{x}; x, y, y; x, \bar{y}, y$ . Three of them are represented in the boundary of the representation domain:  $B = HNP, C = \Gamma NP$  and  $J = \Gamma HP$ ; 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  $\frac{1}{8}$ .

The same result holds for  $(Fm\bar{3})^*$ : the stabilizer is generated by  $2/m..$  and  $t(\frac{1}{2}, \frac{1}{2}, 0) \text{ mod } \mathbf{T}_{\text{int}}$  and is of order 8,  $|\bar{\mathcal{G}}^k| = |\{1\}| = 1$ , the quotient is again  $\frac{1}{8}$ , the parameter range is the same as for  $(Fm\bar{3}m)^*$ . The planes  $H\Gamma_1 P$  and  $N\Gamma_1 P$  are equivalent to  $J = \Gamma HP$  and  $C = \Gamma NP$ , and do not contribute to the parameter ranges.

(3) Plane  $x, y, 0$ : In  $(Fm\bar{3}m)^*$  the stabilizer of plane  $A$  is generated by  $4/mmm$  and  $t(\frac{1}{2}, \frac{1}{2}, 0)$ , order 32,  $\bar{\mathcal{G}}^k$  (site-symmetry group)  $m..$ , order 2. Consequently,  $\Gamma HN$  is  $\frac{1}{16}$  of the unit square  $a^2$ :  $0 < y < x < \frac{1}{2} - y$ . In  $(Fm\bar{3})^*$ , the stabilizer of  $A \cup AA$  is  $mmm$ . plus  $t(\frac{1}{2}, \frac{1}{2}, 0)$ , order 16, with the same group  $\bar{\mathcal{G}}^k$ . Therefore,  $\Gamma H\Gamma_1$  is  $\frac{1}{8}$  of the unit square  $a^2$  in  $(Fm\bar{3})^*$ :  $0 < y < x < \frac{1}{2}$ .

(4) Line  $x, x, 0$ : In  $(Fm\bar{3}m)^*$  the stabilizer is generated by  $m.mm$  and  $t(\frac{1}{2}, \frac{1}{2}, 0) \text{ mod } \mathbf{T}_{\text{int}}$ , order 16,  $\bar{\mathcal{G}}^k$  is  $m.2m$  of order 4. The divisor is 4 and thus  $0 < x < \frac{1}{4}$ . In  $(Fm\bar{3})^*$  the stabilizer is generated by  $2/m..$  and  $t(\frac{1}{2}, \frac{1}{2}, 0) \text{ mod } \mathbf{T}_{\text{int}}$ , order 8, and  $\bar{\mathcal{G}}^k = m..$ , order 2; the divisor is 4 again and  $0 < x < \frac{1}{4}$  is restricted to the same range.†

Data for the independent parameter ranges are essential to make sure that exactly one  $\mathbf{k}$  vector per orbit is represented in the representation domain  $\Phi$  or in the asymmetric unit. Such data are

† Boyle & Kennedy (1988) propose general rules for the parameter ranges of  $\mathbf{k}$ -vector coefficients referred to a primitive basis. The ranges listed in Tables 1.5.5.1 to 1.5.5.4 possibly do not follow these rules.

# 1. GENERAL RELATIONSHIPS AND TECHNIQUES

Table 1.5.5.3. The **k**-vector types for the space groups  $I4/mmm$ ,  $I4/mcm$ ,  $I4_1/amd$  and  $I4_1/acd$

Comparison of the **k**-vector labels and parameters of CDML with the Wyckoff positions of *IT A* for  $I4/mmm$  ( $D_{4h}^{17}$ ), isomorphic to the reciprocal-space group  $\mathcal{G}^*$  of  $4/mmm$ . For the asymmetric unit, see Fig. 1.5.5.3. Two ratios of the lattice constants are distinguished for the representation domains of CDML:  $a > c$  and  $a < c$ , see Figs. 1.5.5.3(a, b) and (c, d). The sign  $\sim$  means symmetrically equivalent. The parameter ranges for the planes and the general position *GP* refer to the asymmetric unit. The coordinates  $x, y, z$  of *IT A* are related to the **k**-vector coefficients of CDML by  $x = 1/2(-k_1 + k_2)$ ,  $y = 1/2(k_1 + k_2 + 2k_3)$ ,  $z = 1/2(k_1 + k_2)$ .

k-vector labels, CDML		Wyckoff position, <i>IT A</i>	Parameters (see Fig. 1.5.5.3), <i>IT A</i>	
$a > c$	$a < c$		$a > c$	$a < c^\dagger$
$\Gamma$ 0, 0, 0	$\Gamma$ 0, 0, 0	$2 a 4/mmm$	0, 0, 0	
$M$ $-\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$M$ $\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}$	$2 b 4/mmm$	$\frac{1}{2}, \frac{1}{2}, 0$	$0, 0, \frac{1}{2}$
$X$ 0, 0, $\frac{1}{2}$	$X$ 0, 0, $\frac{1}{2}$	$4 c mmm$	$0, \frac{1}{2}, 0$	
$P$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$P$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$4 d \bar{4}m2$	$0, \frac{1}{2}, \frac{1}{4}$	
$N$ 0, $\frac{1}{2}, 0$	$N$ 0, $\frac{1}{2}, 0$	$8 f ..2/m$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	
$\Lambda$ $\alpha, \alpha, -\alpha$ $V$ $-\frac{1}{2} + \alpha, \frac{1}{2} + \alpha, \frac{1}{2} - \alpha$	$\Lambda$ $\alpha, \alpha, -\alpha$ —	$4 e 4mm$ $4 e 4mm$	$0, 0, z: 0 < z \leq z_0^\ddagger$ $\frac{1}{2}, \frac{1}{2}, z: 0 < z < z_1 = \frac{1}{2} - z_0$	$0 < z < \frac{1}{2}$ —
$W$ $\alpha, \alpha, \frac{1}{2} - \alpha$	$W$ $\alpha, \alpha, \frac{1}{2} - \alpha$	$8 g 2mm$	$0, \frac{1}{2}, z: 0 < z < \frac{1}{4}$	
$\Sigma$ $-\alpha, \alpha, \alpha$ —	$\Sigma$ $-\alpha, \alpha, \alpha$ $F$ $\frac{1}{2} - \alpha, \frac{1}{2} + \alpha, -\frac{1}{2} + \alpha$	$8 h m.2m$ $8 h m.2m$	$x, x, 0: 0 < x < \frac{1}{2}$ —	$0 < x \leq s_1$ $x, x, \frac{1}{2}: 0 < x < s = \frac{1}{2} - s_1$
$\Delta$ 0, 0, $\alpha$	$\Delta$ 0, 0, $\alpha$	$8 i m2m$	$0, y, 0: 0 < y < \frac{1}{2}$	
$Y$ $-\alpha, \alpha, \frac{1}{2}$ —	$Y$ $-\alpha, \alpha, \frac{1}{2}$ $U$ $\frac{1}{2}, \frac{1}{2}, -\frac{1}{2} + \alpha$	$8 j m2m$ $8 j m2m$	$x, \frac{1}{2}, 0: 0 < x < \frac{1}{2}$ —	$0 < x \leq r$ $0, y, \frac{1}{2}: 0 < y < g = \frac{1}{2} - r$
$Q$ $\frac{1}{4} - \alpha, \frac{1}{4} + \alpha, \frac{1}{4} - \alpha$	$Q$ $\frac{1}{4} - \alpha, \frac{1}{4} + \alpha, \frac{1}{4} - \alpha$	$16 k ..2$	$x, \frac{1}{2} - x, \frac{1}{4}: 0 < x < \frac{1}{4}$	
$C$ $-\alpha, \alpha, \beta$ —	$C$ $-\alpha, \alpha, \beta$ $D$ $\frac{1}{2} - \alpha, \frac{1}{2} + \alpha, -\frac{1}{2} + \beta$	$16 l m..$ $16 l m..$	$x, y, 0: 0 < x < y < \frac{1}{2}\S$ —	— $x, y, \frac{1}{2}$
$B$ $\alpha, \beta, -\alpha$	$B$ $\alpha, \beta, -\alpha$	$16 m ..m$	$x, x, z: 0 < x < \frac{1}{2}, 0 < z < \frac{1}{4} \cup 0 < x < \frac{1}{4}, z = \frac{1}{4}$	
$A$ $\alpha, \alpha, \beta$ $E$ $\alpha - \beta, \alpha + \beta, \frac{1}{2} - \alpha$	$A$ $\alpha, \alpha, \beta$ $E$ $\alpha - \beta, \alpha + \beta, \frac{1}{2} - \alpha$	$16 n .m$ $16 n .m$	$0, y, z: 0 < y < \frac{1}{2}, 0 < z < \frac{1}{2}\P$ $x, \frac{1}{2}, z: \text{transferred to } A = 0, y, z$	
$GP$ $\alpha, \beta, \gamma$	$GP$ $\alpha, \beta, \gamma$	$32 o 1$	$x, y, z: 0 < x < y < \frac{1}{2}, 0 < z < \frac{1}{4} \cup 0 < x < y < \frac{1}{2} - x, z = \frac{1}{4}$	

$\dagger$  If the parameter range is different from that for  $a > c$ .

$\ddagger$   $z_0$  is a coordinate of point  $Z_0$  etc., see Figs. 1.5.5.3(b), (d).

$\S$  For  $a < c$ , the parameter range includes the equivalent of  $D = MSG$ .

$\P$  The parameter range includes  $A$  and the equivalent of  $E$ .

much more difficult to calculate for the representation domains and cannot be found in the cited tables of irreps.

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

(5) Line  $x, x, x$ : In  $(Fm\bar{3}m)^*$  and  $(Fm\bar{3})^*$  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:  $0 < x < \frac{1}{4}, \frac{1}{4} < x < \frac{1}{2}$ .

(6) Plane  $x, x, z$ : In  $(Fm\bar{3}m)^*$  all corners  $\Gamma, N, N_1, H_1$  and all edges are either special points or special lines. Therefore, the parameter ranges are open:  $x, x, z: 0 < x < \frac{1}{4}, 0 < z < \frac{1}{2}$ , where the lines  $x, x, x: 0 \leq x \leq \frac{1}{4}$  and  $x, x, \frac{1}{2} - x: 0 \leq x \leq \frac{1}{4}$  are special lines and thus excepted.

(7) Plane  $x, y, 0$ : In both  $(Fm\bar{3}m)^*$  and  $(Fm\bar{3})^*$ ,  $0 < x$  and  $0 < y$  holds. The **k** vectors of line  $x, x, 0$  have little co-groups of higher order and belong to another Wintgen position in the representation domain (or asymmetric unit) of  $(Fm\bar{3}m)^*$ . Therefore,  $x, y, 0$  is open at its boundary  $x, x, 0$  in the range  $0 < x < \frac{1}{4}$ . In the asymmetric unit

of  $(Fm\bar{3})^*$  the line  $x, x, 0: 0 < x < \frac{1}{4}$  belongs to the plane, in this range the boundary of plane  $A$  is closed. The other range  $x, x, 0: \frac{1}{4} < x < \frac{1}{2}$  is equivalent to the range  $0 < x < \frac{1}{4}$  and thus does not belong to the asymmetric unit; here the boundary of  $AA$  is open.

## 1.5.5.4. Conclusions

As has been shown, *IT A* can serve as a basis for the classification of irreps of space groups by using the concept of reciprocal-space groups:

(a) The asymmetric units of *IT A* are minimal domains of **k** space which are in many cases simpler than the representation domains of the Brillouin zones. However, the asymmetric units of *IT A* are not designed particularly for this use, cf. Section 1.5.4.2. Therefore, it should be checked whether they are the optimal choice for this purpose. Otherwise, other asymmetric units could easily be introduced.

## 1.5. CLASSIFICATION OF SPACE-GROUP REPRESENTATIONS

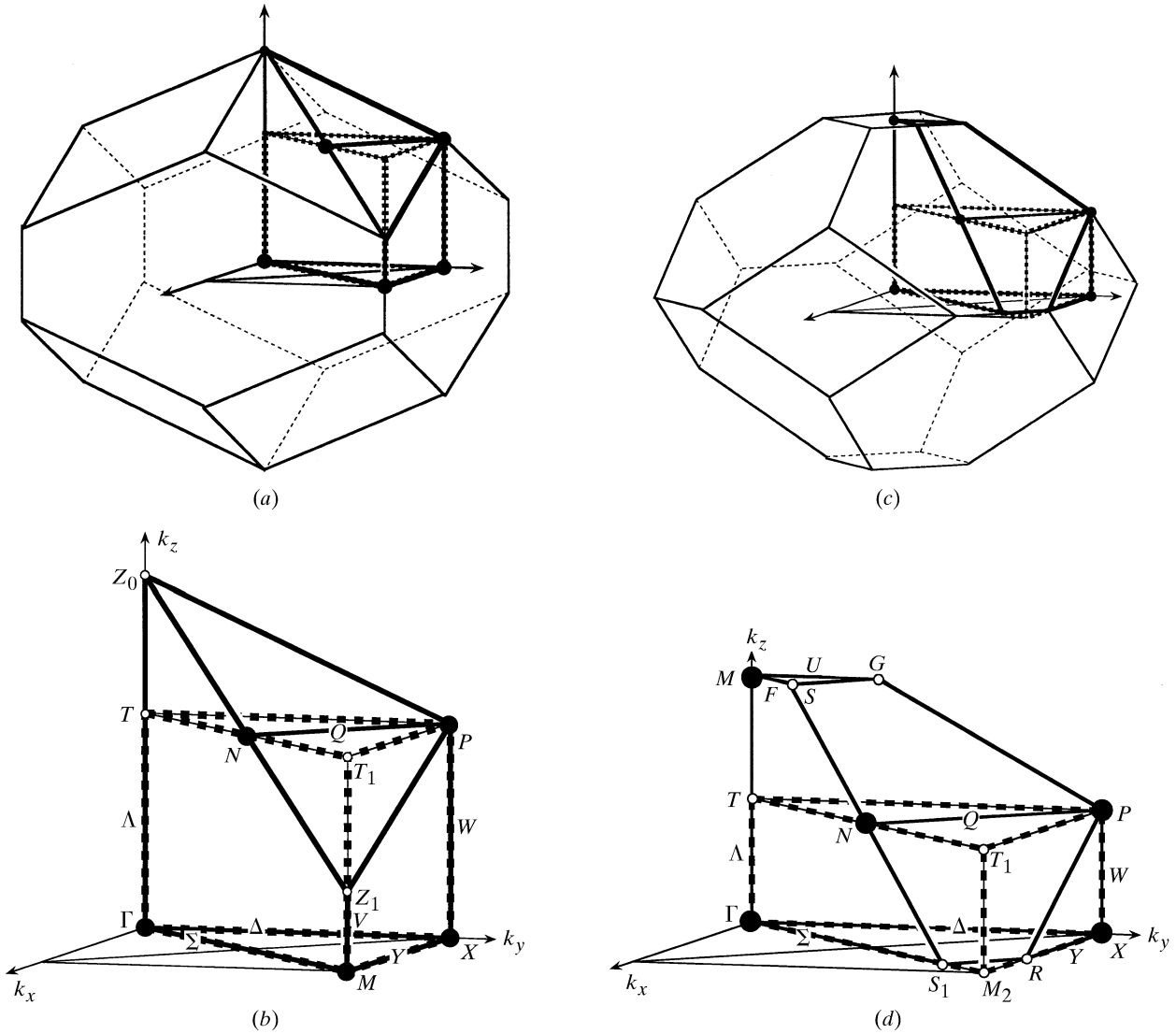


Fig. 1.5.5.3. (a), (b). Symmorphic space group  $I4/mmm$  (isomorphic to the reciprocal-space group  $\mathcal{G}^*$  of  $4/mmmI$ ). Diagrams for  $a > c$ , i.e.  $c^* > a^*$ . In the figures  $a = 1.25c$ , i.e.  $c^* = 1.25a^*$ . (a) Representation domain (thick lines) and asymmetric unit (thick dashed lines, partly protruding) imbedded in the Brillouin zone, which is a tetragonal elongated rhombododecahedron. (b) Representation domain  $\Gamma MXZ_1PZ_0$  and asymmetric unit  $\Gamma MXTT_1P$  of  $I4/mmm$ , IT A, p. 468. The part  $\Gamma MXTNZ_1P$  is common to both bodies; the part  $TNPZ_0$  is equivalent to the part  $NZ_1PT_1$  by a twofold rotation around the axis  $Q = NP$ . Coordinates of the points:  $\Gamma = 0, 0, 0$ ;  $X = 0, \frac{1}{2}, 0$ ;  $M = \frac{1}{2}, \frac{1}{2}, 0$ ;  $P = 0, \frac{1}{2}, \frac{1}{4}$ ;  $N = \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ ;  $T = 0, 0, \frac{1}{4} \sim T_1 = \frac{1}{2}, \frac{1}{2}, \frac{1}{4}$ ;  $Z_0 = 0, 0, z_0 \sim Z_1 = \frac{1}{2}, \frac{1}{2}, z_1$  with  $z_0 = [1 + (c/a)^2]/4$ ;  $z_1 = \frac{1}{2} - z_0$ ; the sign  $\sim$  means symmetrically equivalent. Lines:  $\Lambda = \Gamma Z_0 = 0, 0, z$ ;  $V = Z_1M = \frac{1}{2}, \frac{1}{2}, z$ ;  $W = XP = 0, \frac{1}{2}, z$ ;  $\Sigma = \Gamma M = x, x, 0$ ;  $\Delta = \Gamma X = 0, y, 0$ ;  $Y = XM = x, \frac{1}{2}, 0$ ;  $Q = PN = x, \frac{1}{2} - x, \frac{1}{4}$ . The lines  $Z_0Z_1$ ,  $Z_1P$  and  $PZ_0$  have no special symmetry but belong to special planes. Planes:  $C = \Gamma MX = x, y, 0$ ;  $B = \Gamma Z_0Z_1M = x, x, z$ ;  $A = \Gamma XPZ_0 = 0, y, z$ ;  $E = MXPZ_1 = x, \frac{1}{2}, z$ . The plane  $Z_0Z_1P$  belongs to the general position  $GP$ . Large black circles: special points belonging to the representation domain; small open circles:  $T \sim T_1$  and  $Z_0 \sim Z_1$  belonging to special lines; thick lines: edges of the representation domain and special line  $Q = NP$ ; dashed lines: edges of the asymmetric unit. For the parameter ranges see Table 1.5.5.3.

(c), (d). Symmorphic space group  $I4/mmm$  (isomorphic to the reciprocal-space group  $\mathcal{G}^*$  of  $4/mmmI$ ). Diagrams for  $c > a$ , i.e.  $a^* > c^*$ . In the figures  $c = 1.25a$ , i.e.  $a^* = 1.25c^*$ . (c) Representation domain (thick lines) and asymmetric unit (dashed lines, partly protruding) imbedded in the Brillouin zone, which is a tetragonal cuboctahedron. (d) Representation domain  $\Gamma S_1RXPMSG$  and asymmetric unit  $\Gamma M_2XTT_1P$  of  $I4/mmm$ , IT A, p. 468. The part  $\Gamma S_1RXTNP$  is common to both bodies; the part  $TNPMSG$  is equivalent to the part  $T_1NPM_2S_1R$  by a twofold rotation around the axis  $Q = NP$ . Coordinates of the points:  $\Gamma = 0, 0, 0$ ;  $X = 0, \frac{1}{2}, 0$ ;  $N = \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ ;  $M = 0, 0, \frac{1}{2} \sim M_2 = \frac{1}{2}, \frac{1}{2}, 0$ ;  $T = 0, 0, \frac{1}{4} \sim T_1 = \frac{1}{2}, \frac{1}{2}, \frac{1}{4}$ ;  $P = 0, \frac{1}{2}, \frac{1}{4}$ ;  $S = s, s, \frac{1}{2} \sim S_1 = s_1, s_1, 0$  with  $s = [1 - (a/c)^2]/4$ ;  $s_1 = \frac{1}{2} - s$ ;  $R = r, \frac{1}{2}, 0 \sim G = 0, g, \frac{1}{2}$  with  $r = (a/c)^2/2$ ;  $g = \frac{1}{2} - r$ ; the sign  $\sim$  means symmetrically equivalent. Lines:  $\Lambda = \Gamma M = 0, 0, z$ ;  $W = XP = 0, \frac{1}{2}, z$ ;  $\Sigma = \Gamma S_1 = x, x, 0$ ;  $F = MS = x, x, \frac{1}{2}$ ;  $\Delta = \Gamma X = 0, y, 0$ ;  $Y = XR = x, \frac{1}{2}, 0$ ;  $U = MG = 0, y, \frac{1}{2}$ ;  $Q = PN = x, \frac{1}{2} - x, \frac{1}{4}$ . The lines  $GS \sim S_1R$ ,  $SN \sim NS_1$  and  $GP \sim PR$  have no special symmetry but belong to special planes. Planes:  $C = \Gamma S_1RX = x, y, 0$ ;  $D = MSG = x, y, \frac{1}{2}$ ;  $B = \Gamma S_1SM = x, x, z$ ;  $A = \Gamma XPGM = 0, y, z$ ;  $E = RXP = x, \frac{1}{2}, z$ . The plane  $S_1RPGS$  belongs to the general position  $GP$ . Large black circles: special points belonging to the representation domain; small open circles:  $M_2 \sim M$ ; the points  $T \sim T_1$ ,  $S \sim S_1$  and  $G \sim R$  belong to special lines; thick lines: edges of the representation domain and special line  $Q = NP$ ; dashed lines: edges of the asymmetric unit. For the parameter ranges see Table 1.5.5.3.

# 1. GENERAL RELATIONSHIPS AND TECHNIQUES

Table 1.5.5.4. The **k**-vector types for the space groups *Fmm2* and *Fdd2*

Comparison of the **k**-vector labels and parameters of CDML with the Wyckoff positions of *IT A* for *Imm2* ( $C_{2h}^{20}$ ), isomorphic to the reciprocal-space group  $\mathcal{G}^*$  of *mm2F*. For the asymmetric unit see Fig. 1.5.5.4. Four ratios of the lattice constants are distinguished in CDML, Fig. 3.6 for the representation domains: (a)  $a^{*2} < b^{*2} + c^{*2}$ ,  $b^{*2} < c^{*2} + a^{*2}$  and  $c^{*2} < a^{*2} + b^{*2}$  (see Fig. 1.5.5.4a); (b)  $c^{*2} > a^{*2} + b^{*2}$  (see Fig. 1.5.5.4b); (c)  $b^{*2} > c^{*2} + a^{*2}$  [not displayed because essentially the same as (d)]; (d)  $a^{*2} > b^{*2} + c^{*2}$  (see Fig. 1.5.5.4c). The vertices of the Brillouin zones of Fig. 3.6(a)–(d) with a variable coordinate are not designated in CDML. In Figs. 1.5.5.4 (a), (b) and (c) they are denoted as follows: the end point of the line  $\Lambda$  is  $\Lambda_0$ , of line  $\Delta$  is  $\Delta_0$ , of line  $\Sigma$  is  $\Sigma_0$ , of line  $A$  is  $A_0$  etc. The variable coordinate of the end point is  $\lambda_0$ ,  $\delta_0$ ,  $\sigma_0$ ,  $a_0$  etc., respectively. The line  $A_0B_0$  is called *ab* etc. The plane (111) is called  $\varphi$ . It has the equation in the  $\mathbf{a}^*$ ,  $\mathbf{b}^*$ ,  $\mathbf{c}^*$  basis  $\varphi: a^{*2}x + b^{*2}y + c^{*2}z = d^{*2}/4$  with  $d^{*2} = a^{*2} + b^{*2} + c^{*2}$ . From this equation one calculates the variable coordinates of the vertices of the Brillouin zone:  $\Lambda_0$   $0, 0, \lambda_0$  with  $\lambda_0 = d^{*2}/4c^{*2}$ ;  $Q_0$   $\frac{1}{2}, \frac{1}{2}, q_0$  with  $q_0 = \frac{1}{2} - \lambda_0$ ;  $\Delta_0$   $0, \delta_0, 0$  with  $\delta_0 = d^{*2}/4b^{*2}$ ;  $R_0$   $\frac{1}{2}, r_0, \frac{1}{2}$  with  $r_0 = \frac{1}{2} - \delta_0$ ;  $\Sigma_0$   $\sigma_0, 0, 0$  with  $\sigma_0 = d^{*2}/4a^{*2}$ ;  $U_0$   $u_0, \frac{1}{2}, \frac{1}{2}$  with  $u_0 = \frac{1}{2} - \sigma_0$ ;  $A_0$   $a_0, 0, \frac{1}{2}$  with  $a_0 = \frac{1}{4} + (b^{*2} - c^{*2})/4a^{*2}$ ;  $C_0$   $c_0, \frac{1}{2}, 0$  with  $c_0 = \frac{1}{2} - a_0$ ;  $B_0$   $0, b_0, \frac{1}{2}$  with  $b_0 = \frac{1}{4} + (a^{*2} - c^{*2})/4b^{*2}$ ;  $D_0$   $\frac{1}{2}, d_0, 0$  with  $d_0 = \frac{1}{2} - b_0$ ;  $G_0$   $\frac{1}{2}, 0, g_0$  with  $g_0 = \frac{1}{4} + (b^{*2} - a^{*2})/4c^{*2}$ ;  $H_0$   $0, \frac{1}{2}, h_0$  with  $h_0 = \frac{1}{2} - g_0$ . The coordinates  $x, y, z$  of *IT A* are related to the **k**-vector coefficients of CDML by  $x = 1/2(-k_1 + k_2 + k_3)$ ,  $y = 1/2(k_1 - k_2 + k_3)$ ,  $z = 1/2(k_1 + k_2 - k_3)$ . If necessary, a lattice vector has been added or a twofold screw rotation around the axis  $\frac{1}{4}, \frac{1}{4}, z$  has been performed in order to shift the range of coordinates to  $0 \leq x, y, z \leq \frac{1}{2}$ . For example,  $-\alpha, -\alpha, 0 \sim 0, 0, -z'$  with  $0 < z' < \lambda_0$  is replaced by  $\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z' = \frac{1}{2}, \frac{1}{2}, z$  with  $\frac{1}{2} - \lambda_0 < z < \frac{1}{2}$ . (The sign  $\sim$  means symmetrically equivalent.)

Wyckoff position:  $2 a$  *mm2*. Parameter range in asymmetric unit:  $0, 0, z$  and  $\frac{1}{2}, \frac{1}{2}, z: 0 \leq z < \frac{1}{2}$  (or  $0, 0, z: 0 \leq z < 1$ ).

k-vector label, CDML	Type of Brillouin zone as in:					
	Fig. 1.5.5.4(a)		Fig. 1.5.5.4(b)		Fig. 1.5.5.4(c)	
	CDML	<i>IT A</i>	CDML	<i>IT A</i>	CDML	<i>IT A</i>
$\Gamma$	0, 0, 0	0, 0, 0	0, 0, 0	0, 0, 0	0, 0, 0	0, 0, 0
$Z$	$\frac{1}{2}, \frac{1}{2}, 0$	0, 0, $\frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 1$	$\frac{1}{2}, \frac{1}{2}, 0$	$\frac{1}{2}, \frac{1}{2}, 0$	0, 0, $\frac{1}{2}$
$\Lambda$	$\alpha, \alpha, 0$	0, 0, $z: 0 < z < \frac{1}{2}$	$\alpha, \alpha, 0$	0, 0, $z: 0 < z \leq \lambda_0$	$\alpha, \alpha, 0$	0, 0, $z: 0 < z < \frac{1}{2}$
<i>LE</i>	$-\alpha, -\alpha, 0$	$\frac{1}{2}, \frac{1}{2}, z: 0 < z < \frac{1}{2}$	$-\alpha, -\alpha, 0$	$\frac{1}{2}, \frac{1}{2}, z: \frac{1}{2} - \lambda_0 < z < \frac{1}{2}$	$-\alpha, -\alpha, 0$	$\frac{1}{2}, \frac{1}{2}, z: 0 < z < \frac{1}{2}$
<i>Q</i>			$\frac{1}{2} + \alpha, \frac{1}{2} + \alpha, 1$	$\frac{1}{2}, \frac{1}{2}, z: 0 < z \leq q_0$		
<i>QA</i>			$\frac{1}{2} - \alpha, \frac{1}{2} - \alpha, 1$	0, 0, $z: \frac{1}{2} - q_0 < z < \frac{1}{2}$		

Wyckoff position:  $2 b$  *mm2*. Parameter range in asymmetric unit:  $\frac{1}{2}, 0, z$  and  $0, \frac{1}{2}, z: 0 \leq z < \frac{1}{2}$  (or uni-arm  $\frac{1}{2}, 0, z: 0 \leq z < 1$ ).

k-vector label, CDML	Type of Brillouin zone as in:					
	Fig. 1.5.5.4(a)		Fig. 1.5.5.4(b)		Fig. 1.5.5.4(c)	
	CDML	<i>IT A</i>	CDML	<i>IT A</i>	CDML	<i>IT A</i>
<i>T</i>	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, 0$	$1, \frac{1}{2}, \frac{1}{2}$	$0, \frac{1}{2}, \frac{1}{2}$
<i>Y</i>	$\frac{1}{2}, 0, \frac{1}{2}$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, \frac{1}{2}$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, \frac{1}{2}$	$0, \frac{1}{2}, 0$
<i>G</i>	$\alpha, \frac{1}{2} + \alpha, \frac{1}{2}$	$\frac{1}{2}, 0, z: 0 < z \leq g_0$	$\alpha, \frac{1}{2} + \alpha, \frac{1}{2}$	$\frac{1}{2}, 0, z: 0 < z \leq g_0$		
<i>GA</i>	$-\alpha, \frac{1}{2} - \alpha, \frac{1}{2}$	$0, \frac{1}{2}, z: \frac{1}{2} - g_0 < z < \frac{1}{2}$	$-\alpha, \frac{1}{2} - \alpha, \frac{1}{2}$	$0, \frac{1}{2}, z: \frac{1}{2} - g_0 < z < \frac{1}{2}$		
<i>H</i>	$\frac{1}{2} + \alpha, \alpha, \frac{1}{2}$	$0, \frac{1}{2}, z: 0 < z \leq h_0$	$\frac{1}{2} + \alpha, \alpha, \frac{1}{2}$	$0, \frac{1}{2}, z: 0 < z \leq h_0$	$\frac{1}{2} + \alpha, \alpha, \frac{1}{2}$	$0, \frac{1}{2}, z: 0 < z < \frac{1}{2}$
<i>HA</i>	$\frac{1}{2} - \alpha, -\alpha, \frac{1}{2}$	$\frac{1}{2}, 0, z: \frac{1}{2} - h_0 < z < \frac{1}{2}$	$\frac{1}{2} - \alpha, -\alpha, \frac{1}{2}$	$\frac{1}{2}, 0, z: \frac{1}{2} - h_0 < z < \frac{1}{2}$	$\frac{1}{2} - \alpha, -\alpha, \frac{1}{2}$	$\frac{1}{2}, 0, z: 0 < z < \frac{1}{2}$

(b) All **k**-vector stars giving rise to the same type of irreps belong to the same Wintgen position. In the tables they are collected in one box and are designated by the same Wintgen letter.

(c) The Wyckoff positions of *IT A*, interpreted as Wintgen positions, provide a complete list of the special **k** vectors in the Brillouin zone; the site symmetry of *IT A* is the little co-group  $\bar{G}^{\mathbf{k}}$  of **k**; the multiplicity per primitive unit cell is the number of arms of the star of **k**.

(d) The Wintgen positions with 0, 1, 2 or 3 variable parameters correspond to special **k**-vector points, **k**-vector lines, **k**-vector planes or to the set of all general **k** vectors, respectively.

(e) The complete set of types of irreps is obtained by considering the irreps of one **k** vector per Wintgen position in the uni-arm description or one star of **k** per Wintgen position otherwise. A complete set of inequivalent irreps of  $\mathcal{G}$  is obtained from these irreps by varying the parameters within the asymmetric unit or the representation domain of  $\mathcal{G}^*$ .

(f) For listing each irrep exactly once, the calculation of the parameter range of **k** is often much simpler in the asymmetric unit of the unit cell than in the representation domain of the Brillouin zone.

(g) The consideration of the basic domain  $\Omega$  in relation to the representation domain  $\Phi$  is unnecessary. It may even be misleading, because special **k**-vector subspaces of  $\Omega$  frequently belong to more general types of **k** vectors in  $\Phi$ . 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. If  $\Omega$  is used, and if the representation domain  $\Phi$  is larger than  $\Omega$ , then in most cases the irreps of  $\Phi$  can be obtained from those of  $\Omega$  by extending the parameter ranges of **k**.

(h) The classification by Wintgen letters facilitates the derivation of the correlation tables for the irreps of a group–subgroup chain. The necessary splitting rules for Wyckoff (and thus Wintgen) positions are well known.

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 of *IT A*. Moreover, it is not difficult to relate one approach to the other, see the figures and Tables 1.5.5.1 to 1.5.5.4. The conclusions show that the *crystallographic* approach for the description of irreps of space groups has several advantages as compared to the *traditional*

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Table 1.5.5.4. The **k**-vector types for the space groups *Fmm2* and *Fdd2* (cont.)

Wyckoff position: 4 *c*. *m*. Parameter range in asymmetric unit:  $x, 0, z$  and  $x, \frac{1}{2}, z$ :  $0 < x < \frac{1}{2}$ ;  $0 \leq z < \frac{1}{2}$  (or  $x, 0, z$ :  $0 < x < \frac{1}{2}$ ;  $0 \leq z < 1$ ).

k-vector label, CDML	Type of Brillouin zone as in:					
	Fig. 1.5.5.4(a)		Fig. 1.5.5.4(b)		Fig. 1.5.5.4(c)	
	CDML	IT A	CDML	IT A	CDML	IT A
$\Sigma$	$0, \alpha, \alpha$	$x, 0, 0: 0 < x < \frac{1}{2}$	$0, \alpha, \alpha$	$x, 0, 0: 0 < x < \frac{1}{2}$	$0, \alpha, \alpha$	$x, 0, 0: 0 < x \leq \sigma_0$
<i>U</i>					$1, \frac{1}{2} + \alpha, \frac{1}{2} + \alpha$	$x, 0, 0:$ $\frac{1}{2} - u_0 < x < \frac{1}{2}$
<i>A</i>	$\frac{1}{2}, \frac{1}{2} + \alpha, \alpha$	$x, 0, \frac{1}{2}: 0 < x \leq a_0$			$\frac{1}{2}, \frac{1}{2} + \alpha, \alpha$	$x, 0, \frac{1}{2}: 0 < x \leq a_0$
<i>C</i>	$\frac{1}{2}, \alpha, \frac{1}{2} + \alpha$	$x, 0, \frac{1}{2}: \frac{1}{2} - c_0 < x < \frac{1}{2}$	$\frac{1}{2}, \alpha, \frac{1}{2} + \alpha$	$x, 0, \frac{1}{2}: 0 < x < \frac{1}{2}$	$\frac{1}{2}, \alpha, \frac{1}{2} + \alpha$	$x, 0, \frac{1}{2}:$ $\frac{1}{2} - c_0 < x < \frac{1}{2}$
<i>J</i>	$\alpha, \alpha + \beta, \beta$	$x, 0, z: 0 < x < \frac{1}{2};$ $0 < z < \frac{1}{2}, ga^\dagger$	$\alpha, \alpha + \beta, \beta$	$x, 0, z:$ $0 < x < \frac{1}{2};$ $0 < z \leq \lambda g$	$\alpha, \alpha + \beta, \beta$	$x, 0, z: 0 < z < \frac{1}{2};$ $0 < x \leq \sigma a$
<i>JA</i>	$-\alpha, -\alpha + \beta, \beta$	$x, \frac{1}{2}, z: 0 < x < \frac{1}{2};$ $0, ch < z < \frac{1}{2}$	$-\alpha, -\alpha + \beta, \beta$	$x, \frac{1}{2}, z: 0 < x < \frac{1}{2};$ $qh < z < \frac{1}{2}$	$-\alpha, -\alpha + \beta, \beta$	$x, \frac{1}{2}, z: 0 < z < \frac{1}{2};$ $cu < x < \frac{1}{2}$
<i>K</i>	$\frac{1}{2} + \alpha, \alpha + \beta, \frac{1}{2} + \beta$	$x, \frac{1}{2}, z: 0 < x < c_0;$ $0 < z \leq ch$	$\frac{1}{2} + \alpha, \alpha + \beta, \frac{1}{2} + \beta$	$x, \frac{1}{2}, z: 0 < x < \frac{1}{2};$ $0 < z \leq qh$	$\frac{1}{2} + \alpha, \alpha + \beta,$ $\frac{1}{2} + \beta$	$x, \frac{1}{2}, z: 0 < z < \frac{1}{2};$ $0 < x \leq cu$
<i>KA</i>	$\frac{1}{2} - \alpha, -\alpha + \beta, \frac{1}{2} + \beta$	$x, 0, z:$ $a_0 = \frac{1}{2} - c_0 < x < \frac{1}{2};$ $ga \leq z < \frac{1}{2}$	$\frac{1}{2} - \alpha, -\alpha + \beta, \frac{1}{2} + \beta$	$x, 0, z:$ $0 < x < \frac{1}{2};$ $g\lambda < z < \frac{1}{2}$	$\frac{1}{2} - \alpha, -\alpha + \beta,$ $\frac{1}{2} + \beta$	$x, 0, z: 0 < z < \frac{1}{2};$ $a\sigma < x < \frac{1}{2}$

$\dagger 0 < z < \frac{1}{2}, ga$  means  $0 < z < \text{minimum}(\frac{1}{2} \text{ and } ga)$  where  $ga$  is the line  $G_0A_0$ .

Wyckoff position: 4 *d* *m*... Parameter range in asymmetric unit:  $0, y, z$  and  $\frac{1}{2}, y, z$ :  $0 < y < \frac{1}{2}$ ;  $0 \leq z < \frac{1}{2}$  (or uni-arm  $0, y, z$ :  $0 < y < \frac{1}{2}$ ;  $0 \leq z < 1$ ).

k-vector label, CDML	Type of Brillouin zone as in:					
	Fig. 1.5.5.4(a)		Fig. 1.5.5.4(b)		Fig. 1.5.5.4(c)	
	CDML	IT A	CDML	IT A	CDML	IT A
$\Delta$	$\alpha, 0, \alpha$	$0, y, 0: 0 < y < \frac{1}{2}$	$\alpha, 0, \alpha$	$0, y, 0: 0 < y < \frac{1}{2}$	$\alpha, 0, \alpha$	$0, y, 0: 0 < y < \frac{1}{2}$
<i>B</i>	$\frac{1}{2} + \alpha, \frac{1}{2}, \alpha$	$0, y, \frac{1}{2}: 0 < y \leq b_0$			$\frac{1}{2} + \alpha, \frac{1}{2}, \alpha$	$0, y, \frac{1}{2}: 0 < y < \frac{1}{2}$
<i>D</i>	$\alpha, \frac{1}{2}, \frac{1}{2} + \alpha$	$0, y, \frac{1}{2}:$ $b_0 = \frac{1}{2} - d_0 < y < \frac{1}{2}$	$\alpha, \frac{1}{2}, \frac{1}{2} + \alpha$	$\frac{1}{2}, y, 0: 0 < y < \frac{1}{2}$		
<i>E</i>	$\alpha + \beta, \alpha, \beta$	$0, y, z: 0 < y < \frac{1}{2};$ $0 < z < \frac{1}{2}, hb$	$\alpha + \beta, \alpha, \beta$	$0, y, z:$ $0 < y < \frac{1}{2};$ $0 < z \leq h\lambda$	$\alpha + \beta, \alpha, \beta$	$0, y, z: 0 < y, z < \frac{1}{2}$
<i>EA</i>	$-\alpha + \beta, -\alpha, \beta$	$\frac{1}{2}, y, z: 0 < y < \frac{1}{2};$ $gd, 0 < z < \frac{1}{2}$	$-\alpha + \beta, -\alpha, \beta$	$\frac{1}{2}, y, z: 0 < y < \frac{1}{2};$ $qg < z < \frac{1}{2}$	$-\alpha + \beta, -\alpha, \beta$	$\frac{1}{2}, y, z: 0 < y, z < \frac{1}{2}$
<i>F</i>	$\alpha + \beta, \frac{1}{2} + \alpha, \frac{1}{2} + \beta$	$\frac{1}{2}, y, z: 0 < y < d_0;$ $0 < z \leq dg$	$\alpha + \beta, \frac{1}{2} + \alpha, \frac{1}{2} + \beta$	$\frac{1}{2}, y, z: 0 < y < \frac{1}{2};$ $0 < z \leq qg$		
<i>FA</i>	$-\alpha + \beta, \frac{1}{2} - \alpha, \frac{1}{2} + \beta$	$0, y, z:$ $b_0 = \frac{1}{2} - d_0 < y < \frac{1}{2};$ $hb \leq z < \frac{1}{2}$	$-\alpha + \beta, \frac{1}{2} - \alpha, \frac{1}{2} + \beta$	$0, y, z:$ $0 < y < \frac{1}{2};$ $h\lambda < z < \frac{1}{2}$		

Wyckoff position: (general position) 8 *e* 1 *x, y, z*. Parameter range in asymmetric unit:  $0 < x, y < \frac{1}{2}$ ;  $0 \leq z < \frac{1}{2}$ .

k-vector label, CDML	Type of Brillouin zone as in:					
	Fig. 1.5.5.4(a)		Fig. 1.5.5.4(b)		Fig. 1.5.5.4(c)	
	CDML	IT A	CDML	IT A	CDML	IT A
<i>GP</i>	$\alpha, \beta, \gamma$	$x, y, z$	$\alpha, \beta, \gamma$	$x, y, z$	$\alpha, \beta, \gamma$	$x, y, z$

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 **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 again in order to find the optimal method for the solution of the problem.

The crystallographic approach may be realized in three different ways:

(1) In the *uni-arm description* one lists each **k**-vector star exactly once by indicating the parameter field of the representing **k** vector. Advantages are the transparency of the presentation and the



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relatively small effort required to derive the list. A disadvantage may be that there are protruding flagpoles or wings. Points of these lines or planes 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. Under this approach, all points fulfil the conditions for the asymmetric units of *IT A*, which are always closed. The boundary conditions of *IT A* have to be modified: in reality the boundary is not closed everywhere; there are frequently open parts (see Section 1.5.5.3).

(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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### Appendix 1.5.1.

#### Reciprocal-space groups $\mathcal{G}^*$

This table is based on Table 1 of Wintgen (1941).

In order to obtain the Hermann–Mauguin symbol of  $\mathcal{G}^*$  from that of  $\mathcal{G}$ , one replaces any screw rotations by rotations and any glide reflections by reflections. The result is the symmorphic space group  $\mathcal{G}_0$  assigned to  $\mathcal{G}$ . For most space groups  $\mathcal{G}$ , the reciprocal-space group  $\mathcal{G}^*$  is isomorphic to  $\mathcal{G}_0$ , *i.e.*  $\mathcal{G}^*$  and  $\mathcal{G}$  belong to the same arithmetic crystal class. In the following cases the arithmetic crystal classes of  $\mathcal{G}$  and  $\mathcal{G}^*$  are different, *i.e.*  $\mathcal{G}^*$  can not be obtained in this simple way:

(1) If the lattice symbol of  $\mathcal{G}$  is  $F$  or  $I$ , it has to be replaced by  $I$  or  $F$ . The tetragonal space groups form an exception to this rule; for these the symbol  $I$  persists.

(2) The other exceptions are listed in the following table (for the symbols of the arithmetic crystal classes see *IT A*, Section 8.2.2):

Arithmetic crystal class of $\mathcal{G}$	Reciprocal-space group $\mathcal{G}^*$
$\bar{4}m2I$	$I\bar{4}2m$
$\bar{4}2mI$	$I\bar{4}m2$
$321P$	$P312$
$312P$	$P321$
$3m1P$	$P31m$
$31mP$	$P3m1$
$\bar{3}1mP$	$P\bar{3}m1$
$\bar{3}m1P$	$P\bar{3}1m$
$\bar{6}m2P$	$P\bar{6}2m$
$\bar{6}2mP$	$P\bar{6}m2$