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Table 1.5.4.1. *Conventional coefficients* $(k_i)^T$ *of* **k** *expressed by the adjusted coefficients* (k_{ai}) *of IT A for the different Bravais types of lattices in direct space*

Lattice types	k_1	k_2	k_3
aP, *mP*, *oP*, *tP*, *cP*, *rP*	k_{a1}	k_{a2}	k_{a3}
mA, *oA*	k_{a1}	$2k_{a2}$	$2k_{a3}$
mC, *oC*	$2k_{a1}$	$2k_{a2}$	k_{a3}
oF, *cF*, *oI*, *cI*	$2k_{a1}$	$2k_{a2}$	$2k_{a3}$
tI	$k_{a1} + k_{a2}$	$-k_{a1} + k_{a2}$	$2k_{a3}$
hP	$k_{a1} - k_{a2}$	k_{a2}	k_{a3}
hR (hexagonal)	$2k_{a1} - k_{a2}$	$-k_{a1} + 2k_{a2}$	$3k_{a3}$

Table 1.5.4.2. *Primitive coefficients* $(k_{pi})^T$ *of* **k** *from CDML expressed by the adjusted coefficients* (k_{ai}) *of IT A for the different Bravais types of lattices in direct space*

Lattice types	k_{p1}	k_{p2}	k_{p3}
aP, *mP*, *oP*, *tP*, *cP*, *rP*	k_{a1}	k_{a2}	k_{a3}
mA, *oA*	k_{a1}	$k_{a2}-k_{a3}$	$k_{a2}+k_{a3}$
mC, *oC*	$k_{a1}-k_{a2}$	$k_{a1}+k_{a2}$	k_{a3}
oF, *cF*	$k_{a2}+k_{a3}$	$k_{a1}+k_{a3}$	$k_{a1}+k_{a2}$
oI, *cI*	$-k_{a1}+k_{a2}+k_{a3}$	$k_{a1}-k_{a2}+k_{a3}$	$k_{a1}+k_{a2}-k_{a3}$
tI	$-k_{a1}+k_{a3}$	$k_{a1}+k_{a3}$	$k_{a2}-k_{a3}$
hP	$k_{a1}-k_{a2}$	k_{a2}	k_{a3}
hR (hexagonal)	$k_{a1}+k_{a3}$	$-k_{a1}+k_{a2}+k_{a3}$	$-k_{a2}+k_{a3}$

planes are in many cases much easier to formulate than those for the representation domain.

The **k**-*vector coefficients.* For each **k** vector one can derive a set of irreps of the space group $\mathcal{G}$. Different **k** vectors of a **k** orbit give rise to equivalent irreps. Thus, for the calculation of the irreps of the space groups it is essential to identify the orbits of **k** vectors in reciprocal space. This means finding the sets of all **k** vectors that are related by the operations of the reciprocal-space group $\mathcal{G}^*$ according to equation (1.5.3.13). The classification of these **k** orbits can be done in analogy to that of the point orbits of the symmorphic space groups, as is apparent from the comparison of equations (1.5.3.14) and (1.5.3.15).

The classes of point orbits in direct space under a space group $\mathcal{G}$ are well known and are listed in the space-group tables of *IT* A. They are labelled by *Wyckoff letters*. The stabilizer $\mathcal{S}_{\mathcal{G}}(X)$ of a point X is called the *site-symmetry group* of X, and a *Wyckoff position* consists of all orbits for which the site-symmetry groups are conjugate subgroups of $\mathcal{G}$. Let $\mathcal{G}$ be a symmorphic space group $\mathcal{G}_0$. Owing to the isomorphism between the reciprocal-space groups $\mathcal{G}^*$ and the symmorphic space groups $\mathcal{G}_0$, the complete list of the types of special **k** vectors of $\mathcal{G}^*$ is provided by the Wyckoff positions of $\mathcal{G}_0$. The groups $\mathcal{S}_{\mathcal{G}_0}(X)$ and $\bar{\mathcal{G}}^{\mathbf{k}}$ correspond to each other and the multiplicity of the Wyckoff position (divided by the number of centring vectors per unit cell for centred lattices) equals the number of arms of the star of **k**. Let the vectors **t** of **L** be referred to the conventional basis $(\mathbf{a}_i)^T$ of the space-group tables of *IT* A, as defined in Chapters 2.1 and 9.1 of *IT* A. Then, for the construction of the irreducible representations Γ^k of $\mathcal{T}$ the coefficients of the **k** vectors must be referred to the basis $(\mathbf{a}_j^*)$ of reciprocal space dual to $(\mathbf{a}_i)^T$ in direct space. These **k**-vector coefficients may be different from the conventional coordinates of $\mathcal{G}_0$ listed in the Wyckoff positions of *IT* A.

Example. Let $\mathcal{G}$ be a space group with an *I*-centred cubic lattice **L**, conventional basis $(\mathbf{a}_i)^T$. Then $\mathbf{L}^*$ is an *F*-centred lattice. If referred to the conventional basis $(\mathbf{a}_j^*)$ with $\mathbf{a}_i \cdot \mathbf{a}_j^* = 2\pi\delta_{ij}$, the **k** vectors with coefficients 1 0 0, 0 1 0 and 0 0 1 do not belong to $\mathbf{L}^*$ due to the 'extinction laws' well known in X-ray crystallography. However, in the standard basis of $\mathcal{G}_0$, isomorphic to $\mathcal{G}^*$, the vectors 1 0 0, 0 1 0 and 0 0 1 point to the vertices of the face-centred cube and thus correspond to 2 0 0, 0 2 0 and 0 0 2 referred to the conventional basis $(\mathbf{a}_j^*)$.

In the following, three bases and, therefore, three kinds of coefficients of **k** will be distinguished:

(1) Coefficients referred to the conventional basis $(\mathbf{a}_j^*)$ in reciprocal space, dual to the conventional basis $(\mathbf{a}_i)^T$ in direct space. The corresponding **k**-vector coefficients, $(k_j)^T$, will be called *conventional* coefficients.

(2) Coefficients of **k** referred to a primitive basis $(\mathbf{a}_{pi}^*)$ in reciprocal space (which is dual to a primitive basis in direct space). The corresponding coefficients will be called *primitive* coefficients $(k_{pi})^T$. For a centred lattice the coefficients $(k_{pi})^T$ are different from the conventional coefficients $(k_i)^T$. In most of the physics literature related to space-group representations these primitive coefficients are used, *e.g.* by CDML.

(3) The coefficients of **k** referred to the conventional basis of $\mathcal{G}_0$. These coefficients will be called *adjusted* coefficients $(k_{ai})^T$.

The relations between conventional and adjusted coefficients are listed for the different Bravais types of reciprocal lattices in Table 1.5.4.1, and those between adjusted and primitive coordinates in Table 1.5.4.2. If adjusted coefficients are used, then *IT* A is as suitable for dealing with irreps as it is for handling space-group symmetry.

1.5.4.3. *Wintgen positions*

In order to avoid confusion, in the following the analogues to the Wyckoff positions of $\mathcal{G}_0$ will be called *Wintgen positions* of $\mathcal{G}^*$; the *coordinates* of the Wyckoff position are replaced by the **k**-*vector coefficients* of the Wintgen position, the *Wyckoff letter* will be called the *Wintgen letter*, and the symbols for the *site symmetries* of $\mathcal{G}_0$ are to be read as the symbols for the *little co-groups* $\bar{\mathcal{G}}^{\mathbf{k}}$ of the **k** vectors in $\mathcal{G}^*$. The *multiplicity* of a Wyckoff position is retained in the Wintgen symbol in order to facilitate the use of *IT* A for the description of symmetry in **k** space. However, it is equal to the *multiplicity of the star of* **k** only in the case of primitive lattices $\mathbf{L}^*$.

In analogy to a Wyckoff position, a Wintgen position is a set of orbits of **k** vectors. Each orbit as well as each star of **k** can be represented by any one of its **k** vectors. The zero, one, two or three parameters in the **k**-vector coefficients define points, lines, planes or the full parameter space. The different stars of a Wintgen position are obtained by changing the parameters.

Remark. Because reciprocal space is a vector space, there is no origin choice and the Wintgen letters are unique (in contrast to the Wyckoff letters, which may depend on the origin choice). Therefore, the introduction of *Wintgen sets* in analogy to the *Wyckoff sets* of *IT* A, Section 8.3.2 is not necessary.

It may be advantageous to describe the different stars belonging to a Wintgen position in a *uniform* way. For this purpose one can define:

Definition. Two **k** vectors of a Wintgen position are *uni-arm* if one can be obtained from the other by parameter variation. The *description of the stars* of a Wintgen position is *uni-arm* if the **k** vectors representing these stars are uni-arm.

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 $x = 1/2(k_2 + k_3)$, $y = 1/2(k_1 + k_3)$, $z = 1/2(k_1 + k_2)$.

k-vector label, CDML	Wyckoff position, *IT* A	Parameters (see Fig. 1.5.5.1*b*), *IT* A
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* $m\bar{3}m$	$\frac{1}{2}, 0, 0$
$P\ \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	8 *c* $\bar{4}3m$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$
N 0, 0, $\frac{1}{2}$	24 *d* *m.mm*	$\frac{1}{4}, \frac{1}{4}, 0$
$\Delta\ \alpha, -\alpha, \alpha$	24 *e* 4*m.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. 1.5.5.1*b*) $\sim F_2$ (Fig. 1.5.5.1*b*) $\Lambda \cup F_1 \sim \Gamma H_2 \backslash P$	32 *f* .3*m* 32 *f* .3*m* 32 *f* .3*m* 32 *f* .3*m* 32 *f* .3*m*	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 *g* 2.*mm*	$\frac{1}{4}, \frac{1}{4}, z$: $0 < z < \frac{1}{4}$
Σ 0, 0, α	48 *h* *m.m*2	$x, x, 0$: $0 < x < \frac{1}{4}$
$G\ \frac{1}{2}-\alpha, -\frac{1}{2}+\alpha, \frac{1}{2}$	48 *i* *m.m*2	$\frac{1}{2}-x, x, 0$: $0 < x < \frac{1}{4}$
$A\ \alpha, -\alpha, \beta$	96 *j* *m..*	$x, y, 0$: $0 < y < x < \frac{1}{2}-y$
$B\ \alpha+\beta, -\alpha+\beta, \frac{1}{2}-\beta$ $\sim PH_1N_1$ (Fig. 1.5.5.1*b*) $C\ \alpha, \alpha, \beta$ $J\ \alpha, \beta, \alpha$ $\sim \Gamma PH_1$ (Fig. 1.5.5.1*b*) $C \cup B \cup J \sim \Gamma NN_1H_1$	96 *k* *..m* 96 *k* *..m* 96 *k* *..m* 96 *k* *..m* 96 *k* *..m* 96 *k* *..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 *l* 1	x, y, z: $0 < z < y < x < \frac{1}{2}-y$

For non-holosymmetric space groups the representation domain Φ is a multiple of the basic domain Ω. CDML introduced new letters for stars of **k** vectors in those parts of Φ which do not belong to Ω. If one can make a new **k** vector uni-arm to some **k** vector of the basic domain Ω by an appropriate choice of Φ and Ω, one can extend the parameter range of this **k** vector of Ω to Φ 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 indispensible. 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:†

(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.

† Corresponding tables and figures for all space groups are available at http://www.cryst.ehu.es/cryst/get_kvec.html.