and its reciprocal lattice are always the same. However, there may be differences in the matrix descriptions due to the different orientations of $\mathbf{L}$ and $\mathbf{L}^*$ relative to the symmetry elements of $\bar{\mathcal{G}}$ and due to the reference to the different bases $(\mathbf{a}_i)^T$ and $(\mathbf{a}_i^*)$. For example, if $\mathbf{L}$ has the point symmetry (Hermann–Mauguin symbol) $\bar{3}m1$, then the symbol for the point symmetry of $\mathbf{L}^*$ is $\bar{3}1m$ and *vice versa*.

1.5.3.4. *Irreducible representations of space groups and the reciprocal-space group*

Let $(\mathbf{a}_i)^T$ be a conventional basis of the lattice $\mathbf{L}$ of the space group $\mathcal{G}$. From (1.5.3.6), $k_i = q_i/N_i$ and $\mathbf{k} = \sum_{k=1}^{3} k_i \mathbf{a}_i^*$, equation (1.5.3.4) can be written

$$\Gamma^{q_1 q_2 q_3}[(\boldsymbol{I},\boldsymbol{t})] = \Gamma^{\mathbf{k}}[(\boldsymbol{I},\boldsymbol{t})] = \exp[-i\mathbf{k}\cdot\mathbf{t}]. \qquad (1.5.3.12)$$

Equation (1.5.3.12) has the same form if a primitive basis $(\mathbf{p}_i)^T$ of $\mathbf{L}$ has been chosen. In this case, the vector $\mathbf{k}$ is given by $\mathbf{k} = \sum_{i=1}^{3} k_{pi}\mathbf{p}_i^*$.

Let a primitive basis $(\mathbf{p}_i)^T$ be chosen for the lattice $\mathbf{L}$. The set of all vectors $\mathbf{k}$ (known as wavevectors) forms a discontinuous array. Consider two wavevectors $\mathbf{k}$ and $\mathbf{k}' = \mathbf{k} + \mathbf{K}$, where $\mathbf{K}$ is a vector of the reciprocal lattice $\mathbf{L}^*$. Obviously, $\mathbf{k}$ and $\mathbf{k}'$ describe the same irrep of $\mathcal{T}$. Therefore, to determine all irreps of $\mathcal{T}$ it is necessary to consider only the wavevectors of a small region of the reciprocal space, where the translation of this region by all vectors of $\mathbf{L}^*$ fills the reciprocal space without gap or overlap. Such a region is called a *fundamental region* of $\mathbf{L}^*$. (The nomenclature in literature is not quite uniform. We follow here widely adopted definitions.)

The fundamental region of $\mathbf{L}^*$ is not uniquely determined. Two types of fundamental regions are of interest in this chapter:

(1) The *first Brillouin zone* is that range of $\mathbf{k}$ space around $\mathbf{o}$ for which $|\mathbf{k}| \leq |\mathbf{K} - \mathbf{k}|$ holds for any vector $\mathbf{K} \in \mathbf{L}^*$ (*Wigner–Seitz cell* or *domain of influence* in $\mathbf{k}$ space). The Brillouin zone is used in books and articles on irreps of space groups.

(2) The *crystallographic unit cell in reciprocal space*, for short *unit cell*, is the set of all $\mathbf{k}$ vectors with $0 \leq k_i < 1$. It corresponds to the unit cell used in crystallography for the description of crystal structures in direct space.

Let $\mathbf{k}$ be some vector according to (1.5.3.12) and $\boldsymbol{W}$ be the matrices of $\bar{\mathcal{G}}$. The following definitions are useful:

Definition. The set of all vectors $\mathbf{k}'$ fulfilling the condition

$$\mathbf{k}' = \mathbf{k}\boldsymbol{W} + \mathbf{K}, \quad \boldsymbol{W} \in \bar{\mathcal{G}}, \quad \mathbf{K} \in \mathbf{L}^* \qquad (1.5.3.13)$$

is called *the orbit of* $\mathbf{k}$.

Definition. The set of all matrices $\boldsymbol{W} \in \bar{\mathcal{G}}$ for which

$$\mathbf{k} = \mathbf{k}\boldsymbol{W} + \mathbf{K}, \quad \mathbf{K} \in \mathbf{L}^* \qquad (1.5.3.14)$$

forms a group which is called the *little co-group* $\bar{\mathcal{G}}^{\mathbf{k}}$ of $\mathbf{k}$. The vector $\mathbf{k}$ is called *general* if $\bar{\mathcal{G}}^{\mathbf{k}} = \{\boldsymbol{I}\}$; otherwise $\bar{\mathcal{G}}^{\mathbf{k}} > \{\boldsymbol{I}\}$ and $\mathbf{k}$ is called *special*.

The little co-group $\bar{\mathcal{G}}^{\mathbf{k}}$ is a subgroup of the point group $\bar{\mathcal{G}}$. Consider the coset decomposition of $\bar{\mathcal{G}}$ relative to $\bar{\mathcal{G}}^{\mathbf{k}}$.

Definition. If $\{\boldsymbol{W}_m\}$ is a set of coset representatives of $\bar{\mathcal{G}}$ relative to $\bar{\mathcal{G}}^{\mathbf{k}}$, then the set $\{\mathbf{k}\boldsymbol{W}_m\}$ is called the *star* of $\mathbf{k}$ and the vectors $\mathbf{k}\boldsymbol{W}_m$ are called the *arms of the star*.

The number of arms of the star of $\mathbf{k}$ is equal to the order $|\bar{\mathcal{G}}|$ of the point group $\bar{\mathcal{G}}$ divided by the order $|\bar{\mathcal{G}}^{\mathbf{k}}|$ of the symmetry group $\bar{\mathcal{G}}^{\mathbf{k}}$ of $\mathbf{k}$. If $\mathbf{k}$ is general, then there are $|\bar{\mathcal{G}}|$ vectors from the orbit of $\mathbf{k}$ in each fundamental region and $|\bar{\mathcal{G}}|$ arms of the star. If $\mathbf{k}$ is special with little co-group $\bar{\mathcal{G}}^{\mathbf{k}}$, then the number of arms of the star of $\mathbf{k}$ and the number of $\mathbf{k}$ vectors in the fundamental region from the orbit of $\mathbf{k}$ is $|\bar{\mathcal{G}}\,|/|\bar{\mathcal{G}}^{\mathbf{k}}|$.

Definition. The group of all elements $(\boldsymbol{W},\boldsymbol{w}) \in \mathcal{G}$ for which $\boldsymbol{W} \in \bar{\mathcal{G}}^{\mathbf{k}}$ is called the *little group* $\mathcal{L}^{\mathbf{k}}$ *of* $\mathbf{k}$.

Equation (1.5.3.14) for $\mathbf{k}$ resembles the equation

$$\boldsymbol{x} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{t}, \quad \mathbf{t} \in \mathbf{L} \qquad (1.5.3.15)$$

by which the fixed points of the symmetry operation $(\boldsymbol{W},\boldsymbol{t})$ of a symmorphic space group $\mathcal{G}_0$ are determined. Indeed, the orbits of $\mathbf{k}$ defined by (1.5.3.13) correspond to the point orbits of $\mathcal{G}_0$, the little co-group $\bar{\mathcal{G}}^{\mathbf{k}}$ of $\mathbf{k}$ corresponds to the site-symmetry group of that point $\boldsymbol{X}$ whose coordinates (x_i) have the same values as the vector coefficients $(k_i)^T$ of $\mathbf{k}$, and the star of $\mathbf{k}$ corresponds to a set of representatives of $\boldsymbol{X}$ in $\mathcal{G}_0$. (The analogue of the little group $\mathcal{L}^{\mathbf{k}}$ is rarely considered in crystallography.)

All symmetry operations of $\mathcal{G}_0$ may be obtained as combinations of an operation that leaves the origin fixed with a translation of $\mathbf{L}$, *i.e.* are of the kind $(\boldsymbol{W},\boldsymbol{t}) = (\boldsymbol{I},\boldsymbol{t})(\boldsymbol{W},\boldsymbol{o})$. We now define the analogous group for the $\mathbf{k}$ vectors. Whereas $\mathcal{G}_0$ is a realization of the corresponding abstract group in direct (point) space, the group to be defined will be a realization of it in reciprocal (vector) space.

Definition. The group $\mathcal{G}^*$ which is the semidirect product of the point group $\bar{\mathcal{G}}$ and the translation group of the reciprocal lattice $\mathbf{L}^*$ of $\mathcal{G}$ is called the *reciprocal-space group of* $\mathcal{G}$.

The elements of $\mathcal{G}^*$ are the operations $(\boldsymbol{W},\boldsymbol{K}) = (\boldsymbol{I},\boldsymbol{K})(\boldsymbol{W},\boldsymbol{o})$ with $\boldsymbol{W} \in \bar{\mathcal{G}}$ and $\mathbf{K} \in \mathbf{L}^*$. In order to emphasize that $\mathcal{G}^*$ is a group acting on reciprocal space and not the inverse of a space group (whatever that may mean) we insert a hyphen '-' between 'reciprocal' and 'space'.

From the definition of $\mathcal{G}^*$ it follows that space groups of the same type define the same type of reciprocal-space group $\mathcal{G}^*$. Moreover, as $\mathcal{G}^*$ does not depend on the column parts of the space-group operations, all space groups of the same arithmetic crystal class determine the same type of $\mathcal{G}^*$; for arithmetic crystal class see Section 1.5.3.2. Following Wintgen (1941), the types of reciprocal-space groups $\mathcal{G}^*$ are listed for the arithmetic crystal classes of space groups, *i.e.* for all space groups $\mathcal{G}$, in Appendix 1.5.1.

1.5.4. Conventions in the classification of space-group irreps

Because of the isomorphism between the reciprocal-space groups $\mathcal{G}^*$ and the symmorphic space groups $\mathcal{G}_0$ one can introduce crystallographic conventions in the classification of space-group irreps. These conventions will be compared with those which have mainly been used up to now. Illustrative examples to the following more theoretical considerations are discussed in Section 1.5.5.1.

1.5.4.1. *Fundamental regions*

Different types of regions of reciprocal space may be chosen as fundamental regions, see Section 1.5.3.4. The most frequently used type is the first Brillouin zone, which is the Wigner–Seitz cell (or Voronoi region, Dirichlet domain, domain of influence; *cf. IT* A, Chapter 9.1) of the reciprocal lattice. It has the property that with each $\mathbf{k}$ vector also its star belongs to the Brillouin zone. Such a choice has three advantages:

(1) the Brillouin zone is always primitive and it manifests the point symmetry of the reciprocal lattice $\mathbf{L}^*$ of $\mathcal{G}$;

(2) only **k** vectors of the boundary of the Brillouin zone may have little-group representations which are obtained from projective representations of the little co-group $\bar{\mathcal{G}}^{\mathbf{k}}$, see *e.g.* BC, p. 156;

(3) for physical reasons, the Brillouin zone may be the most convenient fundamental region.

Of these advantages only the third may be essential. For the classification of irreps the minimal domains, see Section 1.5.4.2, are much more important than the fundamental regions. The minimal domain does not display the point-group symmetry anyway and the distinguished **k** vectors always belong to its boundary however the minimal domain may be chosen.

The serious disadvantage of the Brillouin zone is its often complicated shape which, moreover, depends on the lattice parameters of $\mathbf{L}^*$. The body that represents the Brillouin zone belongs to one of the five Fedorov polyhedra (more or less distorted versions of the cubic forms cube, rhombdodecahedron or cuboctahedron, of the hexagonal prism, or of the tetragonal elongated rhombdodecahedron). A more detailed description is that by the 24 *symmetrische Sorten* (Delaunay sorts) of Delaunay (1933), Figs. 11 and 12. According to this classification, the Brillouin zone may display three types of polyhedra of cubic, one type of hexagonal, two of rhombohedral, three of tetragonal, six of orthorhombic, six of monoclinic, and three types of triclinic symmetry.

For low symmetries the shape of the Brillouin zone is so variable that BC, p. 90 *ff.* chose a primitive unit cell of $\mathbf{L}^*$ for the fundamental regions of triclinic and monoclinic crystals. This cell also reflects the point symmetry of $\mathbf{L}^*$, it has six faces only, and although its shape varies with the lattice constants all cells are affinely equivalent. For space groups of higher symmetry, BC and most other authors prefer the Brillouin zone.

Considering $\mathbf{L}^*$ as a lattice, one can refer it to its conventional crystallographic lattice basis. Referred to this basis, the *unit cell of* $\mathbf{L}^*$ is always an alternative to the Brillouin zone. With the exception of the hexagonal lattice, the unit cell of $\mathbf{L}^*$ reflects the point symmetry, it has only six faces and its shape is always affinely equivalent for varying lattice constants. For a space group $\mathcal{G}$ with a primitive lattice, the above-defined conventional unit cell of $\mathbf{L}^*$ is also primitive. If $\mathcal{G}$ has a centred lattice, then $\mathbf{L}^*$ also belongs to a type of centred lattice and the *conventional* cell of $\mathbf{L}^*$ [not to be confused with the cell spanned by the basis $(\mathbf{a}_j^*)$ dual to the basis $(\mathbf{a}_i)^T$] is larger than necessary. However, this is not disturbing because in this context the fundamental region is an auxiliary construction only for the definition of the minimal domain; see Section 1.5.4.2.

1.5.4.2. *Minimal domains*

One can show that all irreps of $\mathcal{G}$ can be built up from the irreps $\Gamma^{\mathbf{k}}$ of $\mathcal{T}$. Moreover, to find all irreps of $\mathcal{G}$ it is only necessary to consider one **k** vector from each orbit of **k**, *cf.* CDML, p. 31.

Definition. A simply connected part of the fundamental region which contains *exactly one* **k** vector of each orbit of **k** is called a *minimal domain* Φ.

The choice of the minimal domain is by no means unique. One of the difficulties in comparing the published data on irreps of space groups is due to the different representation domains found in the literature.

The number of **k** vectors of each general **k** orbit in a fundamental region is always equal to the order of the point group $\bar{\mathcal{G}}$ of $\mathcal{G}$; see Section 1.5.3.4. Therefore, the volume of the minimal domain Φ in reciprocal space is $1/|\bar{\mathcal{G}}|$ of the volume of the fundamental region. Now we can restrict the search for all irreps of $\mathcal{G}$ to the **k** vectors within a minimal domain Φ.

In general, in representation theory of space groups the Brillouin zone is taken as the fundamental region and Φ is called a *representation domain*.† Again, the volume of a representation domain in reciprocal space is $1/|\bar{\mathcal{G}}|$ of the volume of the Brillouin zone. In addition, as the Brillouin zone contains for each **k** vector all **k** vectors of the star of **k**, by application of all symmetry operations $\boldsymbol{W} \in \bar{\mathcal{G}}$ to Φ one obtains the Brillouin zone; *cf.* BC, p. 147. As the Brillouin zone may change its geometrical type depending on the lattice constants, the type of the representation domain may also vary with varying lattice constants; see examples (3) and (4) in Section 1.5.5.1.

The simplest crystal structures are the lattice-like structures that are built up of translationally equivalent points (centres of particles) only. For such a structure the point group $\bar{\mathcal{G}}$ of the space group $\mathcal{G}$ is equal to the point group $\mathcal{Q}$ of its lattice **L**. Such point groups are called *holohedral*, the space group $\mathcal{G}$ is called *holosymmetric*. There are seven holohedral point groups of three dimensions: $\bar{1}, 2/m, mmm, 4/mmm, \bar{3}m, 6/mmm$ and $m\bar{3}m$. For the non-holosymmetric space groups $\mathcal{G}, \bar{\mathcal{G}} < \mathcal{Q}$ holds.

In books on representation theory of space groups, holosymmetric space groups play a distinguished role. Their representation domains are called *basic domains* Ω. For holosymmetric space groups $\Omega = \Phi$ holds. If $\mathcal{G}$ is non-holosymmetric, *i.e.* $\bar{\mathcal{G}} < \mathcal{Q}$ holds, Ω is defined by $\mathcal{Q}$ and is smaller than the representation domain Φ by a factor which is equal to the index of $\bar{\mathcal{G}}$ in $\mathcal{Q}$. In the literature these basic domains are considered to be of primary importance. In Miller & Love (1967) only the irreps for the **k** vectors of the basic domains Ω are listed. Section 5.5 of BC and Davies & Cracknell (1976) state that such a listing is not sufficient for the non-holosymmetric space groups because $\Omega < \Phi$. Section 5.5 of BC shows how to overcome this deficiency; Chapter 4 of CDML introduces new types of **k** vectors for the parts of Φ not belonging to Ω.

The crystallographic analogue of the representation domain in direct space is the *asymmetric unit*, *cf. IT* A. According to its definition it is a simply connected smallest part of space from which by application of all symmetry operations of the space group the whole space is exactly filled. For each space-group type the asymmetric units of *IT* A belong to the same topological type independent of the lattice constants. They are chosen as 'simple' bodies by inspection rather than by applying clearly stated rules. Among the asymmetric units of the 73 symmorphic space-group types $\mathcal{G}_0$ there are 31 parallelepipeds, 27 prisms (13 trigonal, 6 tetragonal and 8 pentagonal) for the non-cubic, and 15 pyramids (11 trigonal and 4 tetragonal) for the cubic $\mathcal{G}_0$.

The asymmetric units of *IT* A – transferred to the groups $\mathcal{G}^*$ of reciprocal space – are alternatives for the representation domains of the literature. They are formulated as closed bodies. Therefore, for inner points **k**, the asymmetric units of *IT* A fulfil the condition that each star of **k** is represented exactly once. For the surface, however, these conditions either have to be worked out or one gives up the condition of uniqueness and replaces *exactly* by *at least* in the definition of the minimal domain (see preceding footnote). The examples of Section 1.5.5.1 show that the conditions for the boundary of the asymmetric unit and its special points, lines and

† From definition 3.7.1 on p. 147 of BC, it does not follow that a representation domain contains *exactly one* **k** vector from each star. The condition 'The intersection of the representation domain with its symmetrically equivalent domains is empty' is missing. Lines 14 to 11 from the bottom of p. 149, however, state that such a property of the representation domain is intended. The representation domains of CDML, Figs. 3.15–3.29 contain *at least one* **k** vector of each star (Vol. 1, pp. 31, 57 and 65). On pp. 66, 67 a procedure is described for eliminating those **k** vectors from the representation domain which occur more than once. In the definition of Altmann (1977), p. 204, the representation domain contains *exactly one* arm (prong) per star.

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 $m\bar{3}ml$. 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
Δ α, $-\alpha$, α	24 *e* 4*m.m*	$x, 0, 0$: $0 < x < \frac{1}{2}$
Λ α, α, α 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 α, α, $\frac{1}{2}-\alpha$	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 α, $-\alpha$, β	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 α, α, β J α, β, α $\sim \Gamma PH_1$ (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 α, β, γ	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.

references