tion 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 $\overline{\mathcal{G}}$ and the translation group of the reciprocal lattice $\mathbf{L}^*$ of $\mathcal{G}$ is called the *reciprocal-space group of* $\mathcal{G}$.

By this definition, the reciprocal-space group $(\mathcal{G})^*$ is isomorphic to a symmorphic space group $\mathcal{G}_0$. The elements of $\mathcal{G}_0$ are the operations $(\boldsymbol{W}, \boldsymbol{t}_{\boldsymbol{K}}) = (\boldsymbol{I}, \boldsymbol{t}_{\boldsymbol{K}})(\boldsymbol{W}, \boldsymbol{o})$ with $\boldsymbol{W} \in \overline{\mathcal{G}}$ and $\boldsymbol{t}_{\boldsymbol{K}} \in \mathbf{L}$ with the coefficients of $\mathbf{K}$. 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 A1.5.1.

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.

1.5.4.1. 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. The Brillouin zone has the property of including the star of each $\mathbf{k}$ vector that belongs to it. Such a choice has three advantages:

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

(2) only $\mathbf{k}$ vectors of the boundary of the Brillouin zone may have little-group representations which are obtained from projective representations of the little co-group $\overline{\mathcal{G}}^{\mathbf{k}}$, 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 $\mathbf{k}$ 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 $\mathbf{L}^*$, *cf.* Section 1.5.5.3. 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*a*,*b*), 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 parameters 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 parameters. 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 $\mathbf{k}$ vector from each orbit of $\mathbf{k}$, *cf.* CDML, p. 31.

Definition. A simply connected part of the fundamental region which contains *exactly one* $\mathbf{k}$ vector of each orbit of $\mathbf{k}$ 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 minimal domains found in the literature.

The number of $\mathbf{k}$ vectors of each general $\mathbf{k}$ orbit in a fundamental region is always equal to the order of the point group $\overline{\mathcal{G}}$ of $\mathcal{G}$; see Section 1.5.3.4. Therefore, the volume of the minimal domain Φ in reciprocal space is $1/|\overline{\mathcal{G}}|$ of the volume of the fundamental region. Now we can restrict the search for all irreps of $\mathcal{G}$ to the $\mathbf{k}$ 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*.[4] Again, the volume of a representation domain in reciprocal space is $1/|\overline{\mathcal{G}}|$ of the volume of the Brillouin zone. In addition, as the Brillouin zone contains for each $\mathbf{k}$ vector all $\mathbf{k}$ vectors of the star of $\mathbf{k}$, by application of all symmetry operations $\boldsymbol{W} \in \overline{\mathcal{G}}$ to Φ one obtains the Brillouin zone; *cf.* BC, p. 147. As the Brillouin zone may change its geometrical type depending on the lattice parameters, the type of the representation domain may also vary with varying lattice parameters; see the examples of Section 1.5.5.

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 $\overline{\mathcal{G}}$ of the space group $\mathcal{G}$ is equal to the point group $\mathcal{Q}$ of its lattice $\mathbf{L}$. Such point groups are called *holohedral*, the space group $\mathcal{G}$ is called *holo-*

[4] From definition 3.7.1 on p. 147 of BC, it does not follow that a representation domain contains *exactly one* $\mathbf{k}$ 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* $\mathbf{k}$ vector of each star (Vol. 1, pp. 31, 57 and 65). On pp. 66, 67 a procedure is described for eliminating those $\mathbf{k}$ 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.

symmetric. There are seven holohedral point groups of three dimensions: $\overline{1}, 2/m, mmm, 4/mmm, \overline{3}m, 6/mmm$ and $m\overline{3}m$. For the non-holosymmetric space groups $\mathcal{G}, \overline{\mathcal{G}} < \mathcal{Q}$ holds. [The group $\mathcal{Q}$ may have *accidentally higher symmetry* in addition, *e.g.* if the lattice of a monoclinic crystal structure is orthorhombic at a certain temperature, pressure and composition. In Section 8.2.6 of *IT* A it is shown how such accidental symmetry can be treated.]

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.* $\overline{\mathcal{G}} < \mathcal{Q}$ 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 $\overline{\mathcal{G}}$ 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 $\mathbf{k}$ 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 labels of $\mathbf{k}$ 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 parameters. 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 $\mathbf{k}$, the asymmetric units of *IT* A fulfil the condition that each star of $\mathbf{k}$ 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 show that the conditions for the boundary of the asymmetric unit and its special points, lines and planes are in many cases much easier to formulate than those for the representation domain. The asymmetric units used here are not always those of *IT* A. They may have been chosen differently in order to make them more convenient for our purpose or to adapt them more or less to the representation domains of CDML.

The $\mathbf{k}$*-vector coefficients.* For each $\mathbf{k}$ vector one can derive a set of irreps of the space group $\mathcal{G}$. Different $\mathbf{k}$ vectors of a $\mathbf{k}$ 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 $\mathbf{k}$ vectors in reciprocal space. This means finding the sets of all $\mathbf{k}$ 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 $\mathbf{k}$ 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 special $\mathbf{k}$ vectors of $(\mathcal{G})^*$ is provided by the Wyckoff positions of $\mathcal{G}_0$. The groups $\mathcal{S}_{\mathcal{G}_0}(X)$ and $\overline{\mathcal{G}}^{\mathbf{k}}$ 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 $\mathbf{k}$. Let the vectors $\mathbf{t}$ of $\mathbf{L}$ 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 irreps $\Gamma^{\mathbf{k}}$ of $\mathcal{T}$ the coefficients of the $\mathbf{k}$ vectors must be referred to the basis $(\mathbf{a}_j^*)$ of reciprocal space dual to $(\mathbf{a}_i)^T$ in direct space. These $\mathbf{k}$-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 $\mathbf{L}$, 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 $\mathbf{k}$ 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 $\mathbf{k}$ 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 $\mathbf{k}$-vector coefficients, $(k_j)^T$, will be called *conventional* coefficients.

(2) Coefficients of $\mathbf{k}$ 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 $\mathbf{k}$ 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 $\mathbf{k}$*-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 cogroups* $\overline{\mathcal{G}}^{\mathbf{k}}$ of the $\mathbf{k}$ 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 $\mathbf{k}$ space. However, it is equal to the *multiplicity of the star of* $\mathbf{k}$ only in the case of primitive lattices $\mathbf{L}^*$.

In analogy to a Wyckoff position, a Wintgen position is a set of orbits of $\mathbf{k}$ vectors. Each orbit as well as each star of $\mathbf{k}$ can be represented by any one of its $\mathbf{k}$ vectors. The zero, one or two free parameters in the $\mathbf{k}$-vector coefficients correspond to special $\mathbf{k}$ vectors, *i.e.*, they define *symmetry points*, *symmetry lines* or *symmetry planes*. Three free parameters indicate general $\mathbf{k}$ vectors. The different stars of a Wintgen position are obtained by varying the free parameters.

For convenience, we call the set of all $\mathbf{k}$ vectors of a Wintgen position a $\mathbf{k}$*-vector type*. A $\mathbf{k}$-vector type consists of complete orbits of $\mathbf{k}$ vectors and thus of full stars of $\mathbf{k}$ vectors; the different orbits of a $\mathbf{k}$-vector type are distinguished by the value(s) of the variable parameter(s) of their $\mathbf{k}$ vectors. Correspondingly, the

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)	$k_{a1}+k_{a3}$	$-k_{a1}+k_{a2}+k_{a3}$	$-k_{a2}+k_{a3}$

irreps belonging to a **k** vector are specified by these parameters and the irreps belonging to a **k**-vector type form a *type of irreps*, Boyle (1986).

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.

The uni-arm description is particularly useful to check whether different sets of **k** vectors belong to the same **k**-vector type or not. Because of the shape of the representation domain or of the asymmetric unit, a **k**-vector type may be split into different parts which belong to different arms of different **k**-vector stars. A uni-arm description may be obtained by the introduction of flagpoles and wings, see Section 1.5.5.1.

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* **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 **k** which is in the unit cell. The order of the little co-group $\overline{\mathcal{G}}^{\mathbf{k}}$ ($\overline{\mathcal{G}}^{\mathbf{k}}$ represents those operations which leave the field of **k** *fixed pointwise*) is divided by the order of the stabilizer of the field in $(\mathcal{G})^*$ [which is the set of all symmetry operations mod (integer translations) which leave the field *invariant as a whole*]. The result gives the independent fraction of the 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. These parameter ranges of the different arms are not necessarily equal, for examples see Section 1.5.5.

Remark. One should avoid the term *equivalent* for the relation between **k** vectors of the same type but with different parameters, as used by Stokes *et al.* (1993) for Λ and *F* or *B*, *C* and *J* of $m\bar{3}mI$, see examples (1) and (2) in Section 1.5.5.4.4. To belong to the same **k**-vector type is only a necessary, not a sufficient, condition for **k**-vector equivalence. On p. 95 of BC is the following definition: 'Two **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 express this by saying: 'Two **k** vectors are equivalent if their difference is a vector **K** of the (reciprocal) lattice'. We prefer to extend this equivalence by saying: 'Two **k** vectors $\mathbf{k}_1$ and $\mathbf{k}_2$ are equivalent if and only if they belong to the same orbit of **k**', *i.e* if there is a matrix part $\boldsymbol{W}$ 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). The **k** vectors of Stokes *et al.* (1993) are not equivalent under this definition, see Davies & Dirl (1987). If the representatives of the **k**-vector stars are chosen uni-arm, their non-equivalence is evident.

It must be mentioned that two **k** vectors of the same type are only called equivalent here if they belong to the same *orbit* of **k** vectors, *i.e.* a **k**-vector type is *not* an equivalence class with respect to the definition of equivalence stated in this remark.

There are two main reasons why **k** vectors of the same type split and then have different labels in CDML:

(1) The higher the symmetry of the point group $\overline{\mathcal{G}}$ of $\mathcal{G}$, the higher is the symmetry of the lattice $\mathbf{L}(\mathcal{G})$ and of the reciprocal lattice $\mathbf{L}^*$, and thus of the Brillouin zone of $\mathcal{G}$. As the symmetry of the Brillouin zone increases, the choice of the boundaries of the representation domain and any other minimal domain becomes more and more restricted. 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. For the arithmetic crystal class $m\bar{3}mI$, for example, all boundary planes, lines and points are fixed, such that all possible minimal domains are equivalent.

For lower point-group symmetries of the fundamental regions, the choice of the minimal domain is less restricted but the Brillouin zones may become more complicated and may even belong to different topological types depending on the ratios of the lattice parameters. Faces and lines on the surface of the Brillouin zone may appear or disappear or change their relative sizes depending on the lattice parameters, causing different descriptions of Wintgen positions.

This does not happen in unit cells or their asymmetric units. Therefore, as already mentioned in Section 1.5.4.1, BC and CDML preferred to replace the different complicated bodies of the Brillouin zones for the possible values of the lattice parameters of the triclinic and monoclinic lattices by the simple primitive unit cells of the reciprocal lattice and to choose the representation domain correspondingly.

(2) For non-holosymmetric space groups the representation domain Φ is a multiple of the basic domain Ω. CDML introduce new letters for **k** vectors which do not belong to Ω. The more symmetry a space group has lost compared to its holosymmetric space group, the more letters of **k** vectors are introduced. The symbols of the basic domain Ω are kept in the names referred to the representation domain Φ. In most cases one can make the new **k** vectors uni-arm to **k** vectors of the basic domain Ω by an appropriate choice of Ω and Φ. Then these **k** vectors belong to the same **k**-vector type and the additional labels can be avoided by *extension of the parameter range* in the **k**-vector space (Boyle, 1986).

Examples where new letters can be avoided by the extension of the parameter range are common, see, *e.g.*, the examples of Section 1.5.5.

In the following example, the introduction of a new name in the transition from a holosymmetric space group to a non-holosymmetric one cannot be avoided because the Wintgen position splits into two positions. We consider the **k** label $Z, \alpha, \frac{1}{2}, 0$ of CDML for the arithmetic crystal class $m\bar{3}mP$, reciprocal-space group $(\mathcal{G})^* = (Pm\bar{3}m)^*$, isomorphic to $Pm\bar{3}m$, Wyckoff position 12 *h* *mm*2 $x, \frac{1}{2}, 0$. In the subgroup $(Pm\bar{3})^*$, this Wintgen position splits into the two positions $\alpha, \frac{1}{2}, 0$ and $\frac{1}{2}, \alpha, 0$, called *Z* and *ZA* by CDML. In the description of *IT* A they are 6 *g* *mm*2 $x, \frac{1}{2}, 0$ and 6 *f* *mm*2 $\frac{1}{2}, x, 0$. In $Pm\bar{3}$, they form two different Wyckoff positions and thus need two different names, as do their Wintgen positions.

references