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1.5. Crystallographic viewpoints in the classification of space-group representations

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1.5.1. List of abbreviations and symbols

BC	Bradley & Cracknell (1972)
CDML	Cracknell, Davies, Miller & Love (1979)
IT A	*International Tables for Crystallography*, Volume A (2005)
irreps	Irreducible representations
L; $\mathbf{L}^*$	Vector lattice of a space group $\mathcal{G}$; reciprocal lattice of $\mathcal{G}$
t	Vector of the lattice **L** of $\mathcal{G}$
k	Vector of the reciprocal space
K	Vector of the reciprocal lattice $\mathbf{L}^*$ [see Note (1)]
a, **b**, **c**; $\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$	Basis vectors of the crystal lattice; basis vectors of the reciprocal lattice
$(\mathbf{a})^T$	Row of basis vectors [see Note (2)]
$(\mathbf{a}^*)$	Column of basis vectors of the reciprocal lattice $\mathbf{L}^*$
X	Point of point space
x, y, z; k_x, k_y, k_z	Point coordinates; vector coefficients
$\boldsymbol{x}$; $\boldsymbol{r}$	Column of point coordinates; column of vector coefficients
$(\boldsymbol{k})^T$	Row of coefficients of a reciprocal-space vector [see Note (2)]
a, b, c	Lengths of the basis vectors of the lattice
α, β, γ	Parameters of **k**-vector coefficients in CDML
a^*, b^*, c^*	Lengths of the basis vectors of the reciprocal lattice
$\boldsymbol{M}$, $\boldsymbol{R}$, $\boldsymbol{D}$, $\boldsymbol{S}$	Matrices
$\boldsymbol{W}$	Matrix part of a mapping
$\boldsymbol{w}$	Column part of a mapping
$(\boldsymbol{A}, \boldsymbol{a})$, $(\boldsymbol{W}, \boldsymbol{w})$	Matrix–column pairs
$\mathcal{G}$; $\mathcal{G}_0$; $(\mathcal{G})^*$	Group or space group; symmorphic space group; reciprocal-space group
$\mathcal{T}$	Translation subgroup of $\mathcal{G}$
$\mathcal{P}$ or $\overline{\mathcal{G}}$; $\mathcal{Q}$	Point group; holohedral point group
$\mathcal{S}$	Site-symmetry group
$\overline{\mathcal{G}}^{\mathbf{k}}$; $\mathcal{L}^{\mathbf{k}}$	Little co-group of **k**; little group of **k**
g, h, e	Group elements of $\mathcal{G}$
2, 3, m	Symmetry operations
$\Gamma(\mathcal{G})$	(Matrix) representation of the group $\mathcal{G}$

Notes: (1) In crystallography, vectors are designated by lower-case bold-face letters. With **K** we make an exception in order to follow the tradition of physics. A crystallographic alternative could be $\mathbf{t}^*$. (2) In crystallography, point coordinates or vector coefficients are written as columns. Therefore, columns are taken as 'normal'. In order to distinguish rows from columns (the coefficients k_i of vectors in reciprocal space, *i.e.* the Miller indices, and the basis of the crystal lattice are written as rows), rows are regarded as transposed columns and are thus marked by $(\ldots)^T$.

1.5.2. Introduction

This chapter on representations widens the scope of the general topics of reciprocal space treated in this volume.

Space-group representations play a growing role in physical applications of crystal symmetry. They are treated in a number of papers and books but comparison of the terms and the listed data is difficult. The main reason for this is the lack of standards in the classification and nomenclature of representations. As a result, the reader is confronted with barely comparable notations used by the different authors, see *e.g.* Stokes & Hatch (1988), Table 7.

The **k** vectors, which can be described as vectors in reciprocal space, play a decisive role in the description and classification of space-group representations. Their symmetry properties are determined by the so-called *reciprocal-space group* $(\mathcal{G})^*$ which is always isomorphic to a symmorphic space group $\mathcal{G}_0$. The different symmetries of **k** vectors correspond to the different kinds of point orbits in the symmorphic space groups $\mathcal{G}_0$. The classification of point orbits into Wyckoff positions in *International Tables for Crystallography* Volume A (*IT* A) (2005) can be used directly to classify the irreducible representations of a space group, abbreviated *irreps*; the Wyckoff positions of the symmorphic space groups $\mathcal{G}_0$ form a basis for a *natural* classification of the irreps. This was first discovered by Wintgen (1941). Similar results have been obtained independently by Raghavacharyulu (1961), who introduced the term reciprocal-space group. In this chapter a classification of irreps is provided which is based on Wintgen's idea.

Although this idea is now more than 60 years old, it has been utilized only rarely and has not yet found proper recognition in the literature and in the existing tables of space-group irreps. Slater (1962) described the correspondence between the special **k** vectors of the Brillouin zone and the Wyckoff positions of space group $Pm\overline{3}m$. Similarly, Jan (1972) compared Wyckoff positions with points of the Brillouin zone when describing the symmetry $Pm\overline{3}$ of the Fermi surface for the pyrite structure. However, the widespread tables of Miller & Love (1967), Zak *et al.* (1969), Bradley & Cracknell (1972) (abbreviated as BC), Cracknell *et al.* (1979) (abbreviated as CDML), and Kovalev (1986) have not made use of this kind of classification and its possibilities, and existing tables are unnecessarily complicated, *cf.* Boyle (1986).

In addition, historical reasons have obscured the classification of irreps and impeded their application. The first considerations of irreps dealt only with space groups of translation lattices (Bouckaert *et al.*, 1936). Later, other space groups were taken into consideration as well. Instead of treating these (lower) symmetries as such, their irreps were derived and classified by starting from the irreps of lattice space groups and proceeding to those of lower symmetry. This procedure has two consequences:

(1) those **k** vectors that are special in a lattice space group are also correspondingly listed in the low-symmetry space group even if they have lost their special properties due to the symmetry reduction;

(2) during the symmetry reduction unnecessary new symbols of **k** vectors are introduced.

The use of the reciprocal-space group $(\mathcal{G})^*$ avoids both these detours.

The relations between the special **k** vectors as listed by CDML and the Wyckoff positions of the space groups of *IT* A have been derived and displayed in figures and tables for a few space groups by Aroyo & Wondratschek (1995). The **k**-vector classification scheme based on Wintgen's (1941) reciprocal-space group approach has been applied meanwhile to all space groups. The compilation of Brillouin-zone figures and **k**-vector correlation tables for the 230 space groups constitutes the wavevector database of the Bilbao Crystallographic Server (1998), a website of crystallographic databases and programs that can be used free

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of charge from any computer with a web browser *via* the Internet (Aroyo, Perez-Mato *et al.*, 2006; Aroyo, Kirov *et al.*, 2006). Simple retrieval tools give direct access to the figures and tables for any space group. The wavevector database available on the server forms the background of the description and classification of the space-group irreps calculated and applied by different programs of the server.

This chapter is a modification of Chapter 1.5 of the second edition of *International Tables for Crystallography*, Volume B, published in 2001. As in the previous edition, we consider in more detail the reciprocal-space group approach and show that widely used crystallographic conventions can be adopted for the classification of space-group representations. Some basic concepts are developed in Section 1.5.3. Possible conventions are discussed in Section 1.5.4. In contrast to Chapter 1.5 in the second edition of *IT* B, the consequences and advantages of the reciprocal-space group approach are demonstrated and discussed in Section 1.5.5 using examples from the database of the Bilbao Crystallographic Server (1998).

1.5.3. Basic concepts

The aim of this section is to give a brief overview of some of the basic concepts related to groups and their representations. Its content should be of some help to readers who wish to refresh their knowledge of space groups and representations, and to familiarize themselves with the kind of description in this chapter. However, it can not serve as an introductory text for these subjects. The interested reader is referred to books dealing with space-group theory, representations of space groups and their applications in solid-state physics: see BC or Chapter 1.2 of *International Tables for Crystallography* Volume D by Janssen (2003).

1.5.3.1. Representations of finite groups

Group theory is the proper tool for studying symmetry in science. The elements of the crystallographic groups are rigid motions (isometries) with regard to performing one after another. The set of all isometries that map an object onto itself always fulfils the group postulates and is called the symmetry or the symmetry group of that object; the isometry itself is called a symmetry operation. Symmetry groups of crystals are dealt with in this chapter. In addition, groups of matrices with regard to matrix multiplication (matrix groups) are considered frequently. Such groups will sometimes be called realizations or representations of abstract groups.

Many applications of group theory to physical problems are closely related to representation theory, *cf.* Rosen (1981) and references therein. In this section, matrix representations Γ of finite groups $\mathcal{G}$ are considered. The concepts of *homomorphism* and *matrix groups* are of essential importance.

A group $\mathcal{B}$ is a homomorphic image of a group $\mathcal{A}$ if there exists a mapping of the elements a_i of $\mathcal{A}$ onto the elements b_k of $\mathcal{B}$ that preserves the multiplication relation (in general several elements of $\mathcal{A}$ are mapped onto one element of $\mathcal{B}$): if $\mathsf{a}_i \rightarrow \mathsf{b}_i$ and $\mathsf{a}_k \rightarrow \mathsf{b}_k$, then $\mathsf{a}_i\mathsf{a}_k \rightarrow \mathsf{b}_i\mathsf{b}_k$ holds for all elements of $\mathcal{A}$ and $\mathcal{B}$ (the image of the product is equal to the product of the images). In the special case of a one-to-one mapping, the homomorphism is called an *isomorphism*.

A matrix group is a group whose elements are non-singular square matrices. The law of combination is matrix multiplication and the group inverse is the inverse matrix. In the following we will be concerned with some basic properties of finite matrix groups relevant to representations.

Let $\mathcal{M}_1$ and $\mathcal{M}_2$ be two matrix groups whose matrices are of the same dimension. They are said to be equivalent if there exists a (non-singular) matrix $\boldsymbol{S}$ such that $\mathcal{M}_2 = \boldsymbol{S}^{-1}\mathcal{M}_1\boldsymbol{S}$ holds. Equivalence implies isomorphism but the inverse is not true: two matrix groups may be isomorphic without being equivalent. According to the theorem of Schur-Auerbach, every finite matrix group is equivalent to a unitary matrix group (by a unitary matrix group we understand a matrix group consisting entirely of unitary matrices).

A matrix group $\mathcal{M}$ is *reducible* if it is equivalent to a matrix group in which every matrix $\boldsymbol{M}$ is of the form

$$\boldsymbol{R} = \begin{pmatrix} \boldsymbol{D}_1 & \boldsymbol{X} \\ \boldsymbol{O} & \boldsymbol{D}_2 \end{pmatrix},$$

see *e.g.* Lomont (1959), p. 47. The group $\mathcal{M}$ is *completely reducible* if it is equivalent to a matrix group in which for all matrices $\boldsymbol{R}$ the submatrices $\boldsymbol{X}$ are $\boldsymbol{O}$ matrices (consisting of zeros only). According to the theorem of Maschke, a finite matrix group is completely reducible if it is reducible. A matrix group is *irreducible* if it is not reducible.

A (matrix) representation $\Gamma(\mathcal{G})$ of a group $\mathcal{G}$ is a homomorphic mapping of $\mathcal{G}$ onto a matrix group $\mathcal{M}(\mathcal{G})$. In a representation Γ every element $\mathsf{g} \in \mathcal{G}$ is associated with a matrix $\boldsymbol{M}(\mathsf{g})$. The dimension of the matrices is called the dimension of the representation.

The above-mentioned theorems on finite matrix groups can be applied directly to representations: we can restrict the considerations to unitary representations only. Further, since every finite matrix group is either completely reducible into irreducible constituents or irreducible, it follows that the infinite set of all matrix representations of a group is known in principle once the irreps are known. Naturally, the question of how to construct all nonequivalent irreps of a finite group and how to classify them arises.

Linear representations are especially important for applications. In this chapter only linear representations of space groups will be considered. Realizations and representations are homomorphic images of abstract groups, but not all of them are linear. In particular, the action of space groups on point space is a nonlinear realization of the abstract space groups because isometries and thus symmetry operations of space groups $\mathcal{G}$ are nonlinear operations. The same holds for their description by matrix-column pairs $(\boldsymbol{W}, \boldsymbol{w})$,[1] by the general position, or by augmented (4×4) matrices, see *IT* A, Part 8. Therefore, the isomorphic matrix representation of a space group, mostly used by crystallographers and listed in the space-group tables of *IT* A as the general position, is not linear.

1.5.3.2. Space groups

In crystallography one deals with real crystals. In many cases the treatment of the crystal is much simpler, but nevertheless describes the crystal and its properties very well, if the real crystal is replaced by an 'ideal crystal'. The real crystal is then considered to be a finite piece of an undisturbed, periodic, and thus infinitely extended arrangement of particles or their centres: ideal crystals are periodic objects in three-dimensional point space E^3, also called direct space. Periodicity means that there are translations among the symmetry operations of ideal crystals. The symmetry group of an ideal crystal is called its space group $\mathcal{G}$.

Space groups $\mathcal{G}$ are of special interest for our problem because:

(1) their irreps are the subject of the classification to be discussed;

(2) this classification makes use of the isomorphism of certain groups to the so-called symmorphic space groups $\mathcal{G}_0$.

Therefore, space groups are introduced here in a slightly more detailed manner than the other concepts. In doing this we follow the definitions and symbolism of *IT* A, Part 8.

[1] In physics written as the Seitz symbol $(\boldsymbol{W}|\boldsymbol{w})$.

To each space group $\mathcal{G}$ belongs an infinite set $\mathcal{T}$ of translations, the *translation subgroup* of $\mathcal{G}$. The group $\mathcal{T}$ forms an infinite Abelian invariant subgroup of $\mathcal{G}$. For each translation its translation vector is defined. The set of all translation vectors is called the *vector lattice* $\mathbf{L}$ of $\mathcal{G}$. Because of the finite size of the atoms constituting the real crystal, the lengths of the translation vectors of the ideal crystal cannot be arbitrarily small; rather there is a lower limit $\delta > 0$ for their length in the range of a few Å.

When referred to a coordinate system $(O, \mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)$, consisting of an origin O and a basis $\mathbf{a}_k$, the symmetry operations, *i.e.* the elements $\mathsf{g}: \tilde{\boldsymbol{x}} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{w}$ of the space group $\mathcal{G}$, are described by matrix–column pairs $(\boldsymbol{W}, \boldsymbol{w})$ with matrix part $\boldsymbol{W}$ and column part $\boldsymbol{w}$. The translations of $\mathcal{G}$ are represented by pairs $(\boldsymbol{I}, \boldsymbol{t}_i)$, where $\boldsymbol{I}$ is the (3×3) unit matrix and $\boldsymbol{t}_i$ is the column of coefficients of the translation vector $\mathbf{t}_i \in \mathbf{L}$. The basis can always be chosen such that all columns $\boldsymbol{t}_i$ and no other columns of translations consist of integers. Such a basis $\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3$ is called a *primitive basis*. For each vector lattice $\mathbf{L}$ there exists an infinite number of primitive bases.

The space group $\mathcal{G}$ can be decomposed into right cosets relative to $\mathcal{T}$:

$$\mathcal{G} = \mathcal{T} \cup \mathcal{T}(\boldsymbol{W}_2, \boldsymbol{w}_2) \cup \ldots \cup \mathcal{T}(\boldsymbol{W}_i, \boldsymbol{w}_i) \cup \ldots \cup \mathcal{T}(\boldsymbol{W}_n, \boldsymbol{w}_n). \quad (1.5.3.1)$$

The coset representatives form the finite set $\mathrm{V} = \{(\boldsymbol{W}_v, \boldsymbol{w}_v)\}$, $v = 1, \ldots, n$, with $(\boldsymbol{W}_1, \boldsymbol{w}_1) = (\boldsymbol{I}, \boldsymbol{o})$, where $\boldsymbol{I}$ is the unit matrix and $\boldsymbol{o}$ is the column consisting of zeros only. The factor group $\mathcal{G}/\mathcal{T}$ is isomorphic to the *point group* $\mathcal{P}$ of $\mathcal{G}$ (called $\overline{\mathcal{G}}$ in books on representation theory) describing the symmetry of the external shape of the macroscopic crystal and being represented by the matrices $\boldsymbol{W}_1, \boldsymbol{W}_2, \ldots, \boldsymbol{W}_n$, $\mathcal{P} = \{\boldsymbol{W}_i\}$. If V can be chosen such that all $\boldsymbol{w}_v = \boldsymbol{o}$, then $\mathcal{G}$ is called a *symmorphic space group* $\mathcal{G}_0$. A symmorphic space group can be recognized easily from its conventional Hermann–Mauguin symbol which does not contain any screw or glide component. In terms of group theory, a symmorphic space group is the semidirect product of $\mathcal{T}$ and $\mathcal{P}$, *cf.* BC, p. 44. In symmorphic space groups $\mathcal{G}_0$ (and in no others) there are site-symmetry groups which are isomorphic to the point group $\mathcal{P}$ of $\mathcal{G}_0$. (For the term 'site-symmetry group', see Section 1.5.4.2.)

Space groups can be classified into 219 (*affine*) *space-group types* either by isomorphism or by affine equivalence; the 230 *crystallographic* space-group types are obtained by restricting the transformations available for affine equivalence to those with positive determinant, *cf. IT* A, Section 8.2.1. Many important properties of space groups are shared by all space groups of a type. In such a case one speaks of *properties of the type.* For example, if a space group is symmorphic, then all space groups of its type are symmorphic, so that one normally speaks of a symmorphic space-group type.

With the concept of symmorphic space groups one can also define the arithmetic crystal classes: Let $\mathcal{G}_0$ be a symmorphic space group referred to a primitive basis and $\mathrm{V} = \{(\boldsymbol{W}_v, \boldsymbol{w}_v)\}$ its set of coset representatives with $\boldsymbol{w}_v = \boldsymbol{o}$ for all columns. To $\mathcal{G}_0$ all those space groups $\mathcal{G}$ can be assigned for which a primitive basis can be found such that the matrix parts $\boldsymbol{W}_v$ of their sets V are the same as those of $\mathcal{G}_0$, only the columns $\boldsymbol{w}_v$ may differ. In this way, to a type of symmorphic space groups $\mathcal{G}_0$, other types of space groups are assigned, *i.e.* the space-group types are classified according to the symmorphic space-group types. These classes are called *arithmetic crystal classes* of space groups or of space-group types.

There are 73 arithmetic crystal classes corresponding to the 73 types of symmorphic space groups; between 1 and 16 space-group types belong to an arithmetic crystal class. A matrix-algebraic definition of arithmetic crystal classes and a proposal for their nomenclature can be found in *IT* A, Section 8.2.3; see also Section 8.3.4 and Table 8.3.4.1.

1.5.3.3. Representations of the translation group $\mathcal{T}$ and the reciprocal lattice

For representation theory we follow the terminology of BC and CDML.

Let $\mathcal{G}$ be referred to a primitive basis. For the following, the infinite set of translations, based on discrete cyclic groups of infinite order, will be replaced by a (very large) finite set in the usual way, assuming the Born–von Karman boundary conditions

$$(\boldsymbol{I}, \boldsymbol{t}_{bi})^{N_i} = (\boldsymbol{I}, N_i) = (\boldsymbol{I}, \boldsymbol{o}) \quad (1.5.3.2)$$

to hold, where $\boldsymbol{t}_{bi} = (1, 0, 0)$, $(0, 1, 0)$ or $(0, 0, 1)$ and N_i is a large integer for $i = 1$, 2 or 3, respectively. Then for any lattice translation $(\boldsymbol{I}, \boldsymbol{t})$,

$$(\boldsymbol{I}, \boldsymbol{N}\boldsymbol{t}) = (\boldsymbol{I}, \boldsymbol{o}) \quad (1.5.3.3)$$

holds, where $\boldsymbol{N}\boldsymbol{t}$ is the column $(N_1 t_1, N_2 t_2, N_3 t_3)$. If the (infinitely many) translations mapped in this way onto $(\boldsymbol{I}, \boldsymbol{o})$ form a normal subgroup $\mathcal{T}_1$ of $\mathcal{G}$, then the mapping described by (1.5.3.3) is a homomorphism. There exists a factor group $\mathcal{G}' = \mathcal{G}/\mathcal{T}_1$ of $\mathcal{G}$ relative to $\mathcal{T}_1$ with translation subgroup $\mathcal{T}' = \mathcal{T}/\mathcal{T}_1$ which is finite and is sometimes called the *finite space group*.

Only the irreps of these finite space groups will be considered. The definitions of space-group type, symmorphic space group *etc.* can be transferred to these groups. Because $\mathcal{T}$ is Abelian, $\mathcal{T}'$ is also Abelian. Replacing the space group $\mathcal{G}$ by $\mathcal{G}'$ means that the especially well developed theory of representations of finite groups can be applied, *cf.* Lomont (1959), Jansen & Boon (1967). For convenience, the prime $'$ will be omitted and the symbol $\mathcal{G}$ will be used instead of $\mathcal{G}'$; $\mathcal{T}'$ will be denoted by $\mathcal{T}$ in the following.

Because $\mathcal{T}$ (formerly $\mathcal{T}'$) is Abelian, its irreps $\Gamma(\mathcal{T})$ are one-dimensional and consist of (complex) roots of unity. Owing to equations (1.5.3.2) and (1.5.3.3), the irreps $\Gamma^{q_1 q_2 q_3}[(\boldsymbol{I}, \boldsymbol{t})]$ of $\mathcal{T}$ have the form

$$\Gamma^{q_1 q_2 q_3}[(\boldsymbol{I}, \boldsymbol{t})] = \exp\left[-2\pi i\left(q_1 \frac{t_1}{N_1} + q_2 \frac{t_2}{N_2} + q_3 \frac{t_3}{N_3}\right)\right], \quad (1.5.3.4)$$

where $\boldsymbol{t}$ is the column (t_1, t_2, t_3), $q_j = 0, 1, 2, \ldots, N_j - 1$, $j = 1, 2, 3$, and t_k and q_j are integers.

Given a primitive basis $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ of $\mathbf{L}$, mathematicians and crystallographers define the *basis of the dual or reciprocal lattice* $\mathbf{L}^*$ by

$$\mathbf{a}_i \cdot \mathbf{a}_j^* = \delta_{ij}, \quad (1.5.3.5)$$

where $\mathbf{a} \cdot \mathbf{a}^*$ is the scalar product between the vectors and δ_{ij} is the unit matrix (see *e.g.* Chapter 1.1, Section 1.1.3). Texts on the physics of solids redefine the basis $\mathbf{a}_1^*, \mathbf{a}_2^*, \mathbf{a}_3^*$ of the *reciprocal lattice* $\mathbf{L}^*$, lengthening each of the basis vectors $\mathbf{a}_j^*$ by the factor 2π. Therefore, in the physicist's convention the relation between the bases of direct and reciprocal lattice reads (*cf.* BC, p. 86):

$$\mathbf{a}_i \cdot \mathbf{a}_j^* = 2\pi\delta_{ij}. \quad (1.5.3.6)$$

In the present chapter only the physicist's basis of the reciprocal lattice is employed, and hence the use of $\mathbf{a}_i^*$ should not lead to misunderstandings. The set of all vectors $\mathbf{K}$,[2]

$$\mathbf{K} = k_1\mathbf{a}_1^* + k_2\mathbf{a}_2^* + k_3\mathbf{a}_3^*, \quad (1.5.3.7)$$

k_i integer, is called the lattice reciprocal to $\mathbf{L}$ or the *reciprocal lattice* $\mathbf{L}^*$.[3]

If one adopts the notation of *IT* A, Part 5, the basis of direct space is denoted by a row $(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)^T$, where $(\,)^T$ means trans-

[2] See Note (1) in Section 1.5.1.

[3] The lattice $\mathbf{L}$ is often called the *direct lattice*. These names are historically introduced and cannot be changed, although equations (1.5.3.5) and (1.5.3.6) show that essentially neither of the lattices is preferred: they form a pair of *mutually reciprocal* lattices.

posed. For reciprocal space, the basis is described by a column $(\mathbf{a}_1^*, \mathbf{a}_2^*, \mathbf{a}_3^*)$.

To each lattice generated from a basis $(\mathbf{a}_i)^T$ a reciprocal lattice is generated from the basis $(\mathbf{a}_j^*)$. Both lattices, $\mathbf{L}$ and $\mathbf{L}^*$, can be compared most easily by referring the direct lattice $\mathbf{L}$ to its *conventional* basis $(\mathbf{a}_i)^T$ as defined in Chapters 2.1 and 9.1 of *IT* A. In this case, the lattice $\mathbf{L}$ may be primitive or centred. If $(\mathbf{a}_i)^T$ forms a primitive basis of $\mathbf{L}$, *i.e.* if $\mathbf{L}$ is primitive, then the basis $(\mathbf{a}_j^*)$ forms a primitive basis of $\mathbf{L}^*$. If $\mathbf{L}$ is centred, *i.e.* $(\mathbf{a}_i)^T$ is not a primitive basis of $\mathbf{L}$, then there exists a centring matrix $\boldsymbol{P}$, $0 < \det(\boldsymbol{P}) < 1$, by which three linearly independent vectors of $\mathbf{L}$ with rational coefficients are generated from those with integer coefficients, *cf. IT* A, Table 5.1.3.1.

Moreover, $\boldsymbol{P}$ can be chosen such that the set of vectors

$$(\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3)^T = (\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)^T \boldsymbol{P} \qquad (1.5.3.8)$$

forms a primitive basis of $\mathbf{L}$. Then the basis vectors $(\mathbf{p}_1^*, \mathbf{p}_2^*, \mathbf{p}_3^*)$ of the lattice reciprocal to the lattice generated by $(\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3)^T$ are determined by

$$(\mathbf{p}_1^*, \mathbf{p}_2^*, \mathbf{p}_3^*) = \boldsymbol{P}^{-1}(\mathbf{a}_1^*, \mathbf{a}_2^*, \mathbf{a}_3^*) \qquad (1.5.3.9)$$

and form a primitive basis of $\mathbf{L}^*$.

Because $\det(\boldsymbol{P}^{-1}) > 1$, not all vectors $\mathbf{K}$ of the form (1.5.3.7) belong to $\mathbf{L}^*$. If k_1, k_2, k_3 are the (integer) coefficients of these vectors $\mathbf{K}$ referred to $(\mathbf{a}_j^*)$ and $k_{p1}\mathbf{p}_1^* + k_{p2}\mathbf{p}_2^* + k_{p3}\mathbf{p}_3^*$ are the vectors of $\mathbf{L}^*$, then $\mathbf{K} = (k_j)^T(\mathbf{a}_j^*) = (k_j)^T\boldsymbol{P}(\mathbf{p}_i^*) = (k_{pi})^T(\mathbf{p}_i^*)$ is a vector of $\mathbf{L}^*$ if and only if the coefficients

$$(k_{p1}, k_{p2}, k_{p3})^T = (k_1, k_2, k_3)^T \boldsymbol{P} \qquad (1.5.3.10)$$

are integers. In other words, $(k_1, k_2, k_3)^T$ has to fulfil the equation

$$(k_1, k_2, k_3)^T = (k_{p1}, k_{p2}, k_{p3})^T \boldsymbol{P}^{-1}. \qquad (1.5.3.11)$$

As is well known, the Bravais type of the reciprocal lattice $\mathbf{L}^*$ is not necessarily the same as that of its direct lattice $\mathbf{L}$. If $\boldsymbol{W}$ is the matrix of a (point-) symmetry operation of the direct lattice, referred to its basis $(\mathbf{a}_i)^T$, then $\boldsymbol{W}^{-1}$ is the matrix of the same symmetry operation of the reciprocal lattice but referred to the dual basis $(\mathbf{a}_i^*)$. This does not affect the symmetry because in a (symmetry) group the inverse of each element in the group also belongs to the group. Therefore, the (point) symmetries of a lattice 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 $\overline{\mathcal{G}}$ 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) $\overline{3}m1$, then the symbol for the point symmetry of $\mathbf{L}^*$ is $\overline{3}1m$ 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 $\mathbf{k} = \sum_{i=1}^{3} k_{pi}\mathbf{p}_i^*$ with rational coefficients k_{pi}.

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). Visually, it is the region of endpoints of the $\mathbf{k}$ vectors that are nearer to the origin than to any other point of the reciprocal lattice. The Brillouin zone is a centrosymmetric body bounded by centrosymmetric planes which bisect perpendicularly the connecting lines from the origin to the neighbouring reciprocal-lattice points. 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 $\overline{\mathcal{G}}$. The following definitions are useful:

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

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

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

Definition. The set of all matrices $\boldsymbol{W} \in \overline{\mathcal{G}}$ 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* $\overline{\mathcal{G}}^{\mathbf{k}}$ of $\mathbf{k}$. The vector $\mathbf{k}$ is called *general* if $\overline{\mathcal{G}}^{\mathbf{k}} = \{\boldsymbol{I}\}$; otherwise $\overline{\mathcal{G}}^{\mathbf{k}} > \{\boldsymbol{I}\}$ and $\mathbf{k}$ is called *special*.

In words: The $\mathbf{k}$ vector is called *general* if its little co-group $\overline{\mathcal{G}}^{\mathbf{k}}$ is the identity of $\overline{\mathcal{G}}$. Otherwise, $\overline{\mathcal{G}}^{\mathbf{k}}$ is a non-trivial subgroup of the point group $\overline{\mathcal{G}}$ of $\mathcal{G}$, $\overline{\mathcal{G}} > \overline{\mathcal{G}}^{\mathbf{k}}$, and $\mathbf{k}$ is called a *special vector* of the reciprocal space.

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 $\overline{\mathcal{G}}^{\mathbf{k}}$ 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 $\mathbf{k}$.

Consider the coset decomposition of $\overline{\mathcal{G}}$ relative to $\overline{\mathcal{G}}^{\mathbf{k}}$.

Definition. If $\{\boldsymbol{W}_m\}$ is a set of coset representatives of $\overline{\mathcal{G}}$ relative to $\overline{\mathcal{G}}^{\mathbf{k}}$, 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 $|\overline{\mathcal{G}}|$ of the point group $\overline{\mathcal{G}}$ divided by the order $|\overline{\mathcal{G}}^{\mathbf{k}}|$ of the symmetry group $\overline{\mathcal{G}}^{\mathbf{k}}$ of $\mathbf{k}$. If $\mathbf{k}$ is general, then there are $|\overline{\mathcal{G}}|$ vectors from the orbit of $\mathbf{k}$ in each fundamental region and $|\overline{\mathcal{G}}|$ arms of the star. If $\mathbf{k}$ is special with little co-group $\overline{\mathcal{G}}^{\mathbf{k}}$, 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 $|\overline{\mathcal{G}}|/|\overline{\mathcal{G}}^{\mathbf{k}}|$.

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

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 transla-

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.

1.5.5. Examples and discussion

The comparison of the crystallographic classification scheme with the traditional one is illustrated by four examples from the Bilbao Crystallographic Server (1998). The examples are designated by the arithmetic crystal classes.

To each arithmetic crystal class of space groups, *cf.* Section 1.5.3.2, there belongs exactly one reciprocal-space group $(\mathcal{G})^*$ which is isomorphic to a type of symmorphic space groups $\mathcal{G}_0$, *cf.* Sections 1.5.3.2 and 1.5.3.4.

(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 $(\mathcal{G})^*$ isomorphic to $Fm\bar{3}m$. The representation domain $\Phi = \Omega$ is equal to the asymmetric unit, see Fig. 1.5.5.1 and Table 1.5.5.1.

(2) **k**-vector types of the arithmetic crystal class $m\bar{3}I$ (space groups $Im\bar{3}$ and $Ia\bar{3}$), reciprocal-space group $(\mathcal{G})^*$ isomorphic to $Fm\bar{3}$. The representation domain $\Phi > \Omega$ is equal to the asymmetric unit; see Fig. 1.5.5.2 and Table 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 $(\mathcal{G})^*$ isomorphic to $I4/mmm$. The representation domains $\Phi = \Omega$ are topologically different for different ratios of the lattice parameters a and c whereas the asymmetric units are affinely equivalent; see Figs. 1.5.5.3 and 1.5.5.4 and Tables 1.5.5.3 and 1.5.5.4.

(4) **k**-vector types of the arithmetic crystal class $mm2F$ ($Fmm2$ and $Fdd2$), reciprocal-space group $(\mathcal{G})^*$ isomorphic to $Imm2$. The representation domains $\Phi > \Omega$ are topologically different for different ratios of the lattice parameters a, b and c whereas the asymmetric units are affinely equivalent; see Figs. 1.5.5.5, 1.5.5.6 and 1.5.5.7, and Tables 1.5.5.5, 1.5.5.6 and 1.5.5.7.

These examples consist essentially of figures and tables. The Brillouin zones with the representation domains of CDML together with the asymmetric units are displayed in the figures. In the synoptic tables the correlation between the **k**-vector tables of CDML and the tables of (Wyckoff) positions in *IT* A is presented. One can thus compare the different descriptions and recognize the relations between them. In addition, the parameter ranges of the **k**-vector types in the asymmetric unit are stated. If a **k**-vector type is listed in the table more than once, then the equivalence relations between the **k** vectors are added such that exactly one representative may be selected for each **k**-vector orbit.

1.5.5.1. Guide to the figures

Each figure caption gives the name of the arithmetic crystal class of space groups to which the Brillouin zone belongs. If there is more than one figure for this arithmetic crystal class, then these figures refer to different geometric conditions for the lattice. Therefore, for each of the figures the arithmetic crystal class is followed by the specific conditions for the lattice parameters of this figure, *e.g.* '$c/a < 1$' for Fig. 1.5.5.3 or '$a^{-2} < b^{-2} + c^{-2}$, $b^{-2} < c^{-2} + a^{-2}$ and $c^{-2} < a^{-2} + b^{-2}$' for Fig. 1.5.5.5.

Then the space groups of the arithmetic crystal class are listed with their Hermann–Mauguin symbols, their Schoenflies symbols and their space-group numbers in *IT* A in parentheses. Following this the type of the reciprocal-space group is denoted, *e.g.* '$(Imm2)^*$, No. 44' for the arithmetic crystal class $mm2F$ in Fig. 1.5.5.5, together with the conditions for the lattice parameters of the reciprocal lattice, if any, and the number of the corresponding table.

The Brillouin zones are objects in reciprocal space. They are displayed in the figures. The reciprocal space is a vector space and its elements are the **k** vectors. Thus the Brillouin zone is a construction in vector space. Because the Brillouin zones are visualized by drawings consisting of vertices, lines and planes, one usually speaks of points, lines and planes in or on the border of the Brillouin zone, not of vectors. Here we follow this tradition.

The Brillouin zones are projected onto the drawing plane by a clinographic projection which may be found *e.g.* in Smith (1982), pp. 61 *f*. The coordinate axes are designated k_x, k_y and k_z; the k_z-coordinate axis points upwards in the projection plane. The diagrams of the Brillouin zones follow those of CDML in order to facilitate the comparison of the data. The origin O with coordinates 0, 0, 0 always forms the centre of the Brillouin zone and is called Γ.

A minimal domain is the smallest fraction of the Brillouin zone which contains *exactly* one wavevector **k** from each orbit. In these examples, the representation domain of CDML is compared with the minimal domain, called 'asymmetric unit', of the Bilbao Crystallographic Server. This asymmetric unit is a simple body and is often chosen in analogy to that of *IT* A. It may coincide with the representation domain of Table 3.10 in CDML, but is mostly rather different. Other than the representation domains of CDML, the asymmetric unit is often *not* fully contained in the Brillouin zone but protrudes from it, in particular by flagpoles and wings, *cf.* the end of this section.

In the figures the edges of the chosen asymmetric unit are drawn into the frame of the Brillouin zone. The names of points, lines and planes of CDML are retained in this listing. New names have been given to points and lines which are not listed in CDML.

The shape of the Brillouin zone depends on the lattice relations. Therefore, there may be vertices of the Brillouin zone with a variable coordinate. If such a point is displayed and designated in a figure by an upper-case letter, then the label of its variable coordinate in the corresponding table is the same letter but lower case. Thus, the variable coordinate of the point G_0 is g_0, of Λ_0 is λ_0 *etc*.

In CDML, the same letter may designate items of different quality in different figures and tables. For example, there is a point H in Fig. 1.5.5.1 and Table 1.5.5.1 but a line H in Fig. 1.5.5.5 and Table 1.5.5.5. In the figures and tables of these examples not only lines and points but also their equivalent objects are listed and the parameter ranges of the lines are described. Therefore, the endpoints of the line H, the points equivalent to a point H as well as the lines equivalent to a line H may be also designated by the letter H but distinguished by indices. In order to recognize points and lines easily, the indices of points are always even: H_0, H_2, H_4; those of lines are always odd: H_1, H_3.

A point is marked in a figure by its name and by a black circle filled with white if it is listed in the corresponding **k**-vector table but is not a point of special symmetry. The same designation is used for the auxiliary points that have been added in order to facilitate the comparison between the two descriptions of the **k**-vector types. Non-coloured parts of the coordinate axes, of the edges of the Brillouin zone or auxiliary lines are displayed by thin solid black lines. Such lines are dashed or omitted if they are not visible, *i.e.* are hidden by the body of the Brillouin zone or of the asymmetric unit.

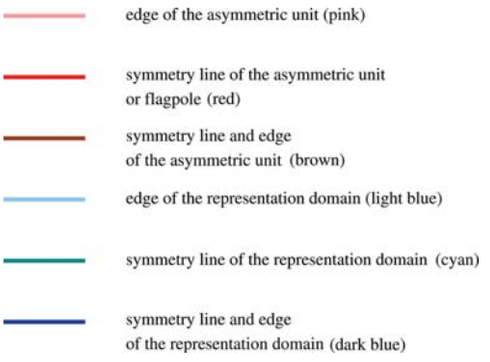
The representatives for the orbits of symmetry points or of symmetry lines, as well as the edges of the representation domain of CDML and of the chosen asymmetric unit are shown in colour.

(*a*) A representative point of each orbit of symmetry points is designated by a red- or cyan-filled circle with its name also in red or cyan if it belongs to the asymmetric unit or to the representation domain of CDML. If both colours could be used, *e.g.* if the asymmetric unit coincides with the representation domain, the colour is red.

Note that a point is coloured red or cyan only if it is really a symmetry *point*, *i.e.* its little co-group is a proper supergroup of the little co-groups of all points in its neighbourhood. Such a point has no variable parameters in its coordinates. Points listed by CDML are not coloured if they are part of a symmetry line or symmetry plane only.

(*b*) Coloured lines are always broad. They are solid lines if they are 'visible', *i.e.* if they are not hidden by the Brillouin zone or by the asymmetric unit. A hidden symmetry line or edge of the asymmetric unit is not suppressed but is coloured as a *dashed line*.

(*c*) The meanings of the different coloured lines and the names used for them in the text are as follows:



Notes:

(1) The colour of the line is pink for an edge of the asymmetric unit which is not a symmetry line.

(2) The colour is red for a symmetry line of the asymmetric unit, with the name also in red.

(3) The colour of the line is brown with the name in red for a line which is a symmetry line as well as an edge of the asymmetric unit.

The representation domain of CDML is displayed in the same figure.

(1) The edges of the representation domain are coloured light blue.

(2) The symmetry points and lines with their letters are coloured cyan.

(3) Edges of the representation domain or common edges of the representation domain and the asymmetric unit are coloured dark blue with the letters in cyan if they are symmetry lines of the representation domain but not of the asymmetric unit.

Common edges of an asymmetric unit and a representation domain are coloured pink if they are not symmetry lines simultaneously.

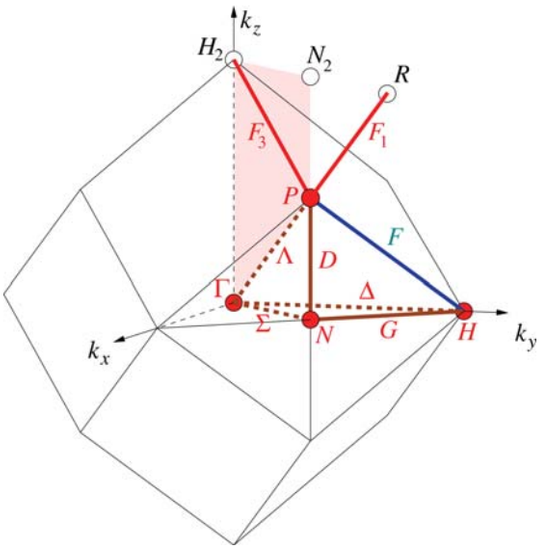


Fig. 1.5.5.1. Brillouin zone with asymmetric unit and representation domain of CDML for arithmetic crystal class $m\bar{3}mI$. Space groups: $Im\bar{3}m - O_h^9$ (229), $Ia\bar{3}d - O_h^{10}$ (230). Reciprocal-space group $(Fm\bar{3}m)$*, No. 225 (see Table 1.5.5.1). The representation domain of CDML is identical with the asymmetric unit. Auxiliary points: R: $\frac{1}{2},\frac{1}{2},\frac{1}{2}$; N_2: $\frac{1}{4},\frac{1}{4},\frac{1}{2}$; H_2: $0,0,\frac{1}{2}$. Flagpole: $F_1 = [P\,R]$ $\quad x,x,x$: $\frac{1}{4} < x < \frac{1}{2}$. Wing: $B_1 \cup J_1 = [\Gamma\,P\,N_2\,H_2]\backslash[F_3]$ $\quad x,x,z$: $0 < x < \frac{1}{4}$; $x < z < \frac{1}{2}$ with $z \neq \frac{1}{2} - x$.

Exactly one element of each point orbit, line orbit or orbit of planes is contained in the asymmetric unit. Exceptionally, *different* elements of the *same* orbit have been coloured because of their special meaning. In these cases the different elements are connected in the corresponding table by the equivalence sign $\sim$, see, *e.g.* the lines $F \sim F_1 = [P\,R]$ or the planes $B \sim B_1 = [P\,N_2\,H_2]$ in Table 1.5.5.1.

To enable a uni-arm description, symmetry lines outside the asymmetric unit may be selected as orbit representatives. Such a piece of a line is called a *flagpole*. Flagpoles are always coloured red, see, *e.g.*, the line F_1 in Fig. 1.5.5.1.

Symmetry planes are not distinguished in the figures. However, in analogy to the flagpoles, symmetry planes outside the asym-

Table 1.5.5.1. *List of* **k***-vector types for arithmetic crystal class* $m\bar{3}mI$

See Fig. 1.5.5.1. Parameter relations: $x = \frac{1}{2}\beta + \frac{1}{2}\gamma$, $y = \frac{1}{2}\alpha + \frac{1}{2}\gamma$, $z = \frac{1}{2}\alpha + \frac{1}{2}\beta$.

k-vector label, CDML	Wyckoff position of *IT* A, *cf.* Section 1.5.4.3	Parameters
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* $m\bar{3}m$	$0,\frac{1}{2},0$
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 $\alpha,-\alpha,\alpha$	24 *e* $4m.m$	$0,y,0$: $0 < y < \frac{1}{2}$
Λ α,α,α	*ex* 32 *f* $.3m$	x,x,x: $0 < x < \frac{1}{4}$
F $\frac{1}{2}-\alpha,-\frac{1}{2}+3\alpha,\frac{1}{2}-\alpha$	*ex* 32 *f* $.3m$	$x,\frac{1}{2}-x,x$: $0 < x < \frac{1}{4}$
$F \sim F_1 = [P\,R]$		x,x,x: $\frac{1}{4} < x < \frac{1}{2}$
$F \sim F_3 = [P\,H_2]$		$x,x,\frac{1}{2}-x$: $0 < x < \frac{1}{4}$
$\Lambda \cup F_1 = [\Gamma R]\backslash[P]$	32 *f* $.3m$	x,x,x: $0 < x < \frac{1}{2}, x \neq \frac{1}{4}$
D $\alpha,\alpha,\frac{1}{2}-\alpha$	48 *g* $2.mm$	$\frac{1}{4},\frac{1}{4},z$: $0 < z < \frac{1}{4}$
Σ $0,0,\alpha$	48 *h* $m.m2$	$x,x,0$: $0 < x < \frac{1}{4}$
G $\frac{1}{2}-\alpha,-\frac{1}{2}+\alpha,\frac{1}{2}$	48 *i* $m.m2$	$x,\frac{1}{2}-x,0$: $0 < x < \frac{1}{4}$
A $\alpha,-\alpha,\beta$	96 *j* $m..$	$x,y,0$: $0 < x < y < \frac{1}{2}-x$
B $\alpha+\beta,-\alpha+\beta,\frac{1}{2}-\beta$	*ex* 96 *k* $..m$	$x,\frac{1}{2}-x,z$: $0 < z < x < \frac{1}{4}$
$B \sim B_1 = [P\,N_2\,H_2]$		x,x,z: $0 < x < \frac{1}{2}-x < z < \frac{1}{2}$
C α,α,β	*ex* 96 *k* $..m$	x,x,z: $0 < z < x < \frac{1}{4}$
J α,β,α	*ex* 96 *k* $..m$	x,y,x: $0 < x < y < \frac{1}{2}-x$
$J \sim J_1 = [\Gamma\,P\,H_2]$		x,x,z: $0 < x < z < \frac{1}{2}-x$
$C \cup B_1 \cup J_1 = [\Gamma\,N\,N_2\,H_2]\backslash[\Lambda,\ F_3]$	96 *k* $..m$	x,x,z: $0 < x < \frac{1}{4}, 0 < z < \frac{1}{2}$ with $z \neq x, z \neq \frac{1}{2}-x$
GP α,β,γ	192 *l* 1	x,y,z: $0 < z < x < y < \frac{1}{2}-x$

metric unit may be selected as orbit representatives. Such a piece of a plane is called a *wing*. Wings are always coloured pink, see, *e.g.*, Fig. 1.5.5.1.

Within the caption of each figure the following data are listed:

(i) a statement of whether the representation domain and the asymmetric unit are identical or not;

(ii) the coordinates of auxiliary points if not specified in the corresponding table;

(iii) the parameter descriptions of the flagpoles and the wings.

1.5.5.2. Guide to the **k***-vector tables*

Each figure is followed by a table with the same number. As for the figures, each table caption gives the name of the arithmetic crystal class of space groups. If there is more than one table for this arithmetic crystal class, then the symbol for the arithmetic crystal class is followed by the specific conditions for the lattice parameters, as for the figures.

Column 1. Label of the **k** vectors in CDML, Tables 3.9 and 3.11 and parameter description of CDML for the set of **k** vectors which belong to the label. No ranges for the parameters are listed in CDML.

If two **k** vectors belong to the same type of **k** vectors, then their little co-groups are conjugate under the reciprocal-space group $(\mathcal{G})^*$ and they correspond to the same Wyckoff position. Different **k** vectors with the *same* CDML label always belong to the same **k**-vector type. **k** vectors with *different* CDML labels may either belong to the same or to different types of **k** vectors. If such **k** vectors belong to the same type, the corresponding Wyckoff-position descriptions are preceded by the letters '*ex*'. Frequently, such **k** vectors have been transformed (sign '$\sim$' in these tables) to equivalent ones in order to make the **k** vectors uni-arm, see the tables in this section.

The parameter range of a region may be described by the vertices of that region in brackets [...]. One point in brackets, *e.g.* [*P*], means the point *P*. Two points within the brackets, *e.g.* [*A B*] means the line from *A* to *B*. Three points within the brackets, *e.g.* [*A B C*] means the triangular region of a plane with the vertices *A*, *B* and *C*. Four or more points may mean a region of a plane or a three-dimensional body, depending on the positions of the points. The meaning can be recognized by studying the corresponding figure. Commas between the points, *e.g.* [*A*, *B*, *C*] indicate the set {*A*, *B*, *C*} of the three points *A*, *B* and *C*.

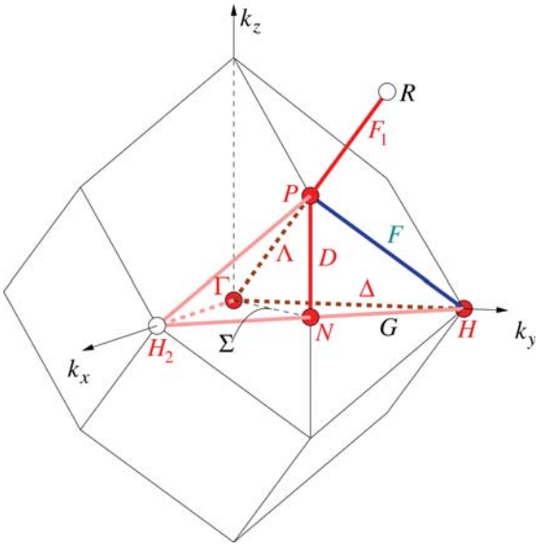


Fig. 1.5.5.2. Brillouin zone with asymmetric unit and representation domain of CDML for arithmetic crystal class $m\bar{3}I$. Space groups $Im\bar{3}-T_h^5$ (204), $Ia\bar{3}-T_h^7$ (206). Reciprocal-space group $(Fm\bar{3})^*$, No. 202 (see Table 1.5.5.2). The representation domain of CDML is identical with the asymmetric unit. Auxiliary points: R: $\frac{1}{2},\frac{1}{2},\frac{1}{2}$; H_2: $\frac{1}{2},0,0$. Flagpole: $F_1=[P\,R]$ x,x,x: $\frac{1}{4}<x<\frac{1}{2}$.

A symbol [...] does not indicate whether the vertices, boundary lines or boundary planes of the region are themselves included or not. All or part of them may belong to the region, all or part of them may not. In the parameter description of the region in Column 3 the inclusion or exclusion is stated by the symbols $\leq$ or $<$.

The backslash '\' is used to indicate included parts not belonging to the described region, see *e.g.* the regions $[\Gamma\,R]\backslash[P]$ and $[\Gamma\,N\,N_2\,H_2]\backslash[\Lambda,\ F_3]$ in Table 1.5.5.1.

Column 2. This column describes the Wyckoff positions (given as the multiplicity, the Wyckoff letter and the site symmetry) of that symmorphic space group $\mathcal{G}_0$ of *IT* A which is isomorphic to the reciprocal-space group $(\mathcal{G})^*$. Each Wyckoff position of $\mathcal{G}_0$ corresponds to a Wintgen position of $(\mathcal{G})^*$, *i.e.* to a type of **k** vectors of $(\mathcal{G})^*$ and *vice versa*.

'Multiplicity' is the number of points in the conventional unit cell of *IT* A. Here it is the number of arms of the star of the **k**

Table 1.5.5.2. *List of* **k***-vector types for arithmetic crystal class* $m\bar{3}I$

See Fig. 1.5.5.2. Parameter relations: $x=\frac{1}{2}\beta+\frac{1}{2}\gamma$, $y=\frac{1}{2}\alpha+\frac{1}{2}\gamma$, $z=\frac{1}{2}\alpha+\frac{1}{2}\beta$.

k-vector label, CDML	Wyckoff position of *IT* A, *cf.* Section 1.5.4.3	Parameters
Γ 0, 0, 0	4 *a* $m\bar{3}$.	0, 0, 0
H $\frac{1}{2},-\frac{1}{2},\frac{1}{2}$	4 *b* $m\bar{3}$.	$0,\frac{1}{2},0$
P $\frac{1}{4},\frac{1}{4},\frac{1}{4}$	8 *c* 23.	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$
N $0,0,\frac{1}{2}$	24 *d* 2/*m*..	$\frac{1}{4},\frac{1}{4},0$
Δ $\alpha,-\alpha,\alpha$	24 *e* *mm*2..	$0,y,0$: $0<y<\frac{1}{2}$
Λ α,α,α	*ex* 32 *f* .3.	x,x,x: $0<x<\frac{1}{4}$
F $\frac{1}{2}-\alpha,-\frac{1}{2}+3\alpha,\frac{1}{2}-\alpha$	*ex* 32 *f* .3.	$x,\frac{1}{2}-x,x$: $0<x<\frac{1}{4}$
$F\sim F_1=[P\,R]$		x,x,x: $\frac{1}{4}<x<\frac{1}{2}$
$\Lambda\cup F_1\sim[\Gamma\,R]\backslash[P]$	32 *f* .3.	x,x,x: $0<x<\frac{1}{2}$, $x\neq\frac{1}{4}$
D $\alpha,\alpha,\frac{1}{2}-\alpha$	48 *g* 2..	$\frac{1}{4},\frac{1}{4},z$: $0<z<\frac{1}{4}$
Σ $0,0,\alpha$	*ex* 48 *h* *m*..	$x,x,0$: $0<x<\frac{1}{4}$
G $\frac{1}{2}-\alpha,-\frac{1}{2}+\alpha,\frac{1}{2}$	*ex* 48 *h* *m*..	$x,\frac{1}{2}-x,0$: $0<x<\frac{1}{4}$
$A=[\Gamma\,N\,H]$ $\alpha,-\alpha,\beta$	*ex* 48 *h* *m*..	$x,y,0$: $0<x<y<\frac{1}{2}-x$
$AA=[\Gamma\,H_2\,N]$ $-\alpha,\alpha,\beta$	*ex* 48 *h* *m*..	$x,y,0$: $0<y<x<\frac{1}{2}-y$
$\Sigma\cup G\cup A\cup AA$	48 *h* *m*..	$x,y,0$: $0<y<\frac{1}{2}-x<\frac{1}{2}\cup$ $\cup\ x,\frac{1}{2}-x,0$: $0<x<\frac{1}{4}$
GP α,β,γ	96 *i* 1	x,y,z: $0<z\leq x<y<\frac{1}{2}-x\cup$ $\cup\ x,y,z$: $0<z<y<x\leq\frac{1}{2}-y\cup$ $\cup\ x,x,z$: $0<z<x<\frac{1}{4}$

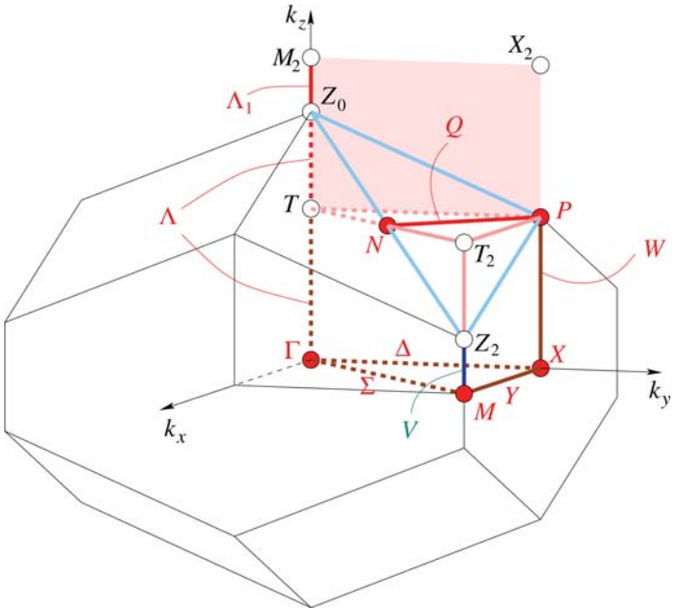


Fig. 1.5.5.3. Brillouin zone with asymmetric unit and representation domain of CDML for arithmetic crystal class $4/mmmI$: $c/a<1$. Space groups $I4/mmm-D_{4h}^{17}$ (139) to $I4_1/acd-D_{4h}^{20}$ (142). Reciprocal-space group $(I4/mmm)$*, No. 139: $c^*/a^*>1$ (see Table 1.5.5.3). The representation domain of CDML is different from the asymmetric unit. Auxiliary points: T: $0,0,\frac{1}{4}$; T_2: $\frac{1}{2},\frac{1}{2},\frac{1}{4}$; X_2: $0,\frac{1}{2},\frac{1}{2}$. Flagpole: $[T\,M_2]$ $\quad 0,0,z$: $\frac{1}{4}<z<\frac{1}{2}$. Wing: $[T\,P\,X_2\,M_2]$ $\quad 0,y,z$: $0<y<\frac{1}{2}$, $\frac{1}{4}<z<\frac{1}{2}$.

vector, multiplied by the number of centring vectors of the conventional unit cell in *IT* A.

Unlike in *IT* A, each table starts with the Wyckoff letter *a* for a Wyckoff position of highest site symmetry and proceeds in alphabetical order until the general position *GP* is reached. The sequence of the CDML labels is not that of CDML but is determined essentially by the alphabetical sequence of the Wyckoff positions.

The symbol for the site symmetry is 'oriented', as given in the space-group tables of *IT* A. For the nomenclature, see Section 2.2.12 of *IT* A.

Column 3. These are the parameters of that Wyckoff position of $\mathcal{G}_0$ which corresponds to the **k**-vector label in CDML, see Column 1. The *parameter description* and the *parameter range* are listed. This range is chosen such that each orbit of the Wyckoff position of *IT* A, *i.e.* also each **k**-vector orbit, is listed exactly once.

The following designation is used for the parameter ranges:

(1) The statement $0<x,\ y<\frac{1}{2}$ means that x and y may vary independently from 0 to $\frac{1}{2}$, 0 and $\frac{1}{2}$ both excluded.

(2) The statement

$$GP \quad \alpha,\beta,\gamma \quad 48\ h\ 1 \quad x,y,z\colon 0\le z<x<y<\tfrac{1}{2} \ \cup \ \cup\ x,\tfrac{1}{2},z\colon 0<z<x<\tfrac{1}{2}$$

means that the description of the asymmetric unit is split into two adjacent regions, a body and a plane. The boundary plane $z=0$ of the body is included, all other boundaries are excluded. Together the regions contain exactly one representative for each **k**-vector orbit of the general position *GP* of the reciprocal-space group.

(3) The statement $x,\frac{1}{2},z\colon -x<z\le x,\ z\ne 0$ means that z may assume any value between $-x$ and $+x$, $z=x$ included but $z=-x$ and $z=0$ excluded.

(4) Occasionally the parameter description becomes too clumsy. Then the data listed are abbreviated by replacing the parametrical data by the designation of the corresponding region.

Table 1.5.5.3. *List of* ***k****-vector types for arithmetic crystal class* $4/mmmI$: $c/a<1$

See Fig. 1.5.5.3. Wyckoff positions *e* and *f* exchanged. Parameter relations: $x=-\frac{1}{2}\alpha+\frac{1}{2}\beta$, $y=\frac{1}{2}\alpha+\frac{1}{2}\beta+\gamma$, $z=\frac{1}{2}\alpha+\frac{1}{2}\beta$.

k-vector label, CDML	Wyckoff position of *IT* A, *cf.* Section 1.5.4.3				Parameters
$\Gamma\quad 0,0,0$		2	*a*	$4/mmm$	$0,0,0$
$M\quad -\frac{1}{2},\frac{1}{2},\frac{1}{2}$		2	*b*	$4/mmm$	$\frac{1}{2},\frac{1}{2},0$
$M\sim M_2$					$0,0,\frac{1}{2}$
$X\quad 0,0,\frac{1}{2}$		4	*c*	$mmm.$	$0,\frac{1}{2},0$
$P\quad \frac{1}{4},\frac{1}{4},\frac{1}{4}$		4	*d*	$\bar{4}m2$	$0,\frac{1}{2},\frac{1}{4}$
$N\quad 0,\frac{1}{2},0$		8	*f*	$..2/m$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$
$\Lambda\quad \alpha,\alpha,-\alpha$	*ex*	4	*e*	$4mm$	$0,0,z$: $0<z\le z_0$
$V\quad -\frac{1}{2}+\alpha,\frac{1}{2}+\alpha,\frac{1}{2}-\alpha$	*ex*	4	*e*	$4mm$	$\frac{1}{2},\frac{1}{2},z$: $0<z<z_2=\frac{1}{2}-z_0$
$V\sim\Lambda_1=[Z_0\,M_2]$					$0,0,z$: $z_0<z<\frac{1}{2}$
$\Lambda\cup\Lambda_1=[\Gamma\,M_2]$		4	*e*	$4mm$	$0,0,z$: $0<z<\frac{1}{2}$
$W\quad \alpha,\alpha,\frac{1}{2}-\alpha$		8	*g*	$2mm.$	$0,\frac{1}{2},z$: $0<z<\frac{1}{4}$
$\Sigma\quad -\alpha,\alpha,\alpha$		8	*h*	$m.2m$	$x,x,0$: $0<x<\frac{1}{2}$
$\Delta\quad 0,0,\alpha$		8	*i*	$m2m.$	$0,y,0$: $0<y<\frac{1}{2}$
$Y\quad -\alpha,\alpha,\frac{1}{2}$		8	*j*	$m2m.$	$x,\frac{1}{2},0$: $0<x<\frac{1}{2}$
$Q\quad \frac{1}{4}-\alpha,\frac{1}{4}+\alpha,\frac{1}{4}-\alpha$		16	*k*	$..2$	$x,\frac{1}{2}-x,\frac{1}{4}$: $0<x<\frac{1}{4}$
$C\quad -\alpha,\alpha,\beta$		16	*l*	$m..$	$x,y,0$: $0<x<y<\frac{1}{2}$
$B\quad \alpha,\beta,-\alpha$		16	*m*	$..m$	x,x,z: $[\Gamma\,M\,Z_2\,Z_0]$
$B=B_1\cup B_2$ $=[\Gamma\,M\,Z_2\,N\,T]\cup[T\,N\,Z_0]$					
$B_2\sim B_3$					x,x,z: $[N\,Z_2\,T_2]$
$B_1\cup B_3=[\Gamma\,M\,T_2\,T]$		16	*m*	$..m$	x,x,z: $0<x<\frac{1}{2},\ 0<z<\frac{1}{4}\ \cup$ $\cup\ x,x,\frac{1}{4}$: $0<x<\frac{1}{4}$
$A\quad \alpha,\alpha,\beta$	*ex*	16	*n*	$.m.$	$0,y,z$: $[\Gamma\,X\,P\,Z_0]$
$E\quad \alpha-\beta,\alpha+\beta,\frac{1}{2}-\alpha$	*ex*	16	*n*	$.m.$	$x,\frac{1}{2},z$: $[M\,X\,P\,Z_2]$
$E\sim A_1$					$0,y,z$: $[P\,X_2\,M_2\,Z_0]$
$A\cup A_1=[\Gamma\,X\,X_2\,M_2]$		16	*n*	$.m.$	$0,y,z$: $0<y,z<\frac{1}{2}$
$GP\quad \alpha,\beta,\gamma$		32	*o*	1	x,y,z: $0<x<y<\frac{1}{2}$; $0<z<\frac{1}{4}\ \cup$ $\cup\ x,y,\frac{1}{4}$: $0<x<y<\frac{1}{2}-x$

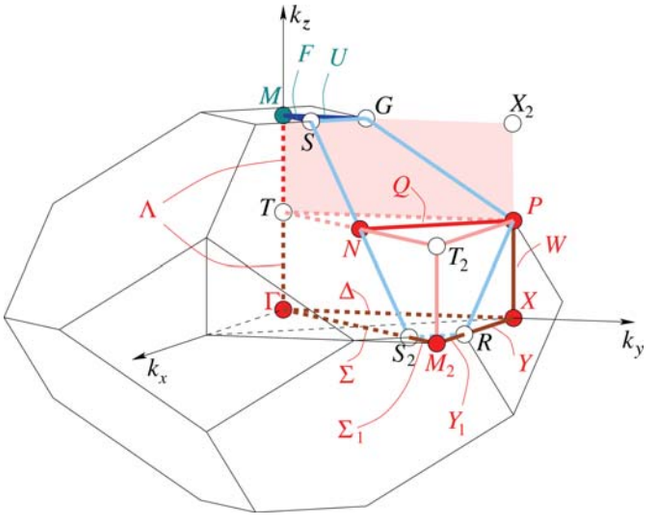


Fig. 1.5.5.4. Brillouin zone with asymmetric unit and representation domain of CDML for arithmetic crystal class $4/mmmI$: $c/a>1$. Space groups $I4/mmm-D_{4h}^{17}$ (139) to $I4_1/acd-D_{4h}^{20}$ (142). Reciprocal-space group $(I4/mmm)$*, No. 139: $c^*/a^*<1$ (see Table 1.5.5.4). The representation domain of CDML is different from the asymmetric unit. Auxiliary points: X_2: $0,\frac{1}{2},\frac{1}{2}$; T: $0,0,\frac{1}{4}$; T_2: $\frac{1}{2},\frac{1}{2},\frac{1}{4}$. Flagpole: $[T\,M]$ $0,0,z$: $\frac{1}{4}<z<\frac{1}{2}$. Wing: $[T\,P\,X_2\,M]$ $0,y,z$: $0<y<\frac{1}{2}, \frac{1}{4}<z<\frac{1}{2}$.

Example. In Table 1.5.5.3 one finds for the arithmetic crystal class $4/mmmI$ of space groups:

$$B\quad \alpha,\beta,-\alpha\quad 16\ m\ ..m\quad x,x,z\text{: }[\Gamma\,M\,Z_2\,Z_0]$$

The parameter description would be:

$$x,x,z\text{: }0<x<\tfrac{1}{2},\ 0<z\le z_0-2x(2z_0-\tfrac{1}{2})$$

Horizontal lines. The horizontal lines extending across the tables separate blocks with different numbers of free parameters. Decisive for this subdivision is the number of free parameters of the Wyckoff position to which the Wintgen position is assigned, not the number of free parameters of CDML.

Example. Arithmetic crystal class mm2F, see Table 1.5.5.5

The **k**-vector labels 'Γ $0,0,0$' and 'Z $\frac{1}{2},\frac{1}{2},0$' of CDML have no free parameter. However, they correspond to the Wyckoff position '2 *a mm*2 $0,0,z$', which has one free parameter. Therefore, Γ and Z are listed together with 'Λ $\alpha,\alpha,0$' and 'LE $-\alpha,-\alpha,0$' in the block for the symmetry lines, *i.e.* for the **k** vectors with one free parameter: in $(Imm2)$* there is no parameter-free Wintgen position at all. The **k**-vector labels 'Σ $0,\alpha,\alpha$' and 'A $\frac{1}{2},\frac{1}{2}+\alpha,\alpha$' of CDML have one free parameter each. However, they correspond together with other **k**-vector labels to the Wyckoff position '4 *c .m.* $x,0,z$'. Therefore, Σ and A are listed together with 'J $\alpha,\alpha+\beta,\beta$' and '$JA$ $-\alpha,-\alpha+\beta,\beta$' and others in the block for the planes, *i.e.* for the **k** vectors with two free parameters.

Table 1.5.5.4. *List of* **k***-vector types for arithmetic crystal class* $4/mmmI$: $c/a>1$

See Fig. 1.5.5.4. Wyckoff positions e and f exchanged. Parameter relations: $x=-\frac{1}{2}\alpha+\frac{1}{2}\beta$, $y=\frac{1}{2}\alpha+\frac{1}{2}\beta+\gamma$, $z=\frac{1}{2}\alpha+\frac{1}{2}\beta$.

k-vector label, CDML	Wyckoff position of *IT* A, *cf.* Section 1.5.4.3	Parameters
Γ $0,0,0$	2 a $4/mmm$	$0,0,0$
M $\frac{1}{2},\frac{1}{2},-\frac{1}{2}$	2 b $4/mmm$	$0,0,\frac{1}{2}$
$M\sim M_2$		$\frac{1}{2},\frac{1}{2},0$
X $0,0,\frac{1}{2}$	4 c $mmm.$	$0,\frac{1}{2},0$
P $\frac{1}{4},\frac{1}{4},\frac{1}{4}$	4 d $\bar{4}m2$	$0,\frac{1}{2},\frac{1}{4}$
N $0,\frac{1}{2},0$	8 f $..2/m$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$
Λ $\alpha,\alpha,-\alpha$	4 e $4mm$	$0,0,z$: $0<z<\frac{1}{2}$
W $\alpha,\alpha,\frac{1}{2}-\alpha$	8 g $2mm.$	$0,\frac{1}{2},z$: $0<z<\frac{1}{4}$
Σ $-\alpha,\alpha,\alpha$	*ex* 8 h $m.2m$	$x,x,0$: $0<x\le s_2$
F $\frac{1}{2}-\alpha,\frac{1}{2}+\alpha,-\frac{1}{2}+\alpha$	*ex* 8 h $m.2m$	$x,x,\frac{1}{2}$: $0<x<s=\frac{1}{2}-s_2$
$F\sim\Sigma_1=[S_2\,M_2]$		$x,x,0$: $s_2<x<\frac{1}{2}$
$\Sigma\cup\Sigma_1=[\Gamma M_2]$	8 h $m.2m$	$x,x,0$: $0<x<\frac{1}{2}$
Δ $0,0,\alpha$	8 i $m2m.$	$0,y,0$: $0<y<\frac{1}{2}$
Y $-\alpha,\alpha,\frac{1}{2}$	*ex* 8 j $m2m.$	$x,\frac{1}{2},0$: $0<x\le r$
U $\frac{1}{2},\frac{1}{2},-\frac{1}{2}+\alpha$	*ex* 8 j $m2m.$	$0,y,\frac{1}{2}$: $0<y<g=\frac{1}{2}-r$
$U\sim Y_1=[R\,M_2]$		$x,\frac{1}{2},0$: $r<x<\frac{1}{2}$
$Y\cup Y_1=[X\,M_2]$	8 j $m2m.$	$x,\frac{1}{2},0$: $0<x<\frac{1}{2}$
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 $-\alpha,\alpha,\beta$	*ex* 16 l $m..$	$x,y,0$: $[\Gamma\,S_2\,R\,X]$
D $\frac{1}{2}-\alpha,\frac{1}{2}+\alpha,-\frac{1}{2}+\beta$	*ex* 16 l $m..$	$x,y,\frac{1}{2}$: $[M\,S\,G]$
$D\sim C_1$		$x,y,0$: $[M_2\,R\,S_2]$
$C\cup C_1=[\Gamma\,M_2\,X]$	16 l $m..$	$x,y,0$: $0<x<y<\frac{1}{2}$
B $\alpha,\beta,-\alpha$	16 m $..m$	x,x,z: $[\Gamma\,S_2\,S\,M]$
$B=B_1\cup B_2$ $=[\Gamma\,S_2\,N\,T]\cup[T\,N\,S\,M]$		
$B_2\sim B_3$		x,x,z: $[T_2\,N\,S_2\,M_2]$
$B_1\cup B_3=[\Gamma\,M_2\,T_2\,T]$	16 m $..m$	x,x,z: $0<x<\frac{1}{2}, 0<z<\frac{1}{4}\cup$ $\cup\,x,x,\frac{1}{4}$: $0<x<\frac{1}{4}$
A α,α,β	*ex* 16 n $.m.$	$0,y,z$: $[\Gamma\,X\,P\,G\,M]$
E $\alpha-\beta,\alpha+\beta,\frac{1}{2}-\alpha$	*ex* 16 n $.m.$	$x,\frac{1}{2},z$: $[X\,P\,R]$
$E\sim A_1$		$0,y,z$: $[X_2\,G\,P]$
$A\cup A_1=[\Gamma\,X\,X_2\,M]$	16 n $.m.$	$0,y,z$: $0<y,z<\frac{1}{2}$
GP α,β,γ	32 o 1	x,y,z: $0<x<y<\frac{1}{2}$; $0<z<\frac{1}{4}\cup$ $\cup\,x,y,\frac{1}{4}$: $0<x<y<\frac{1}{2}-x$

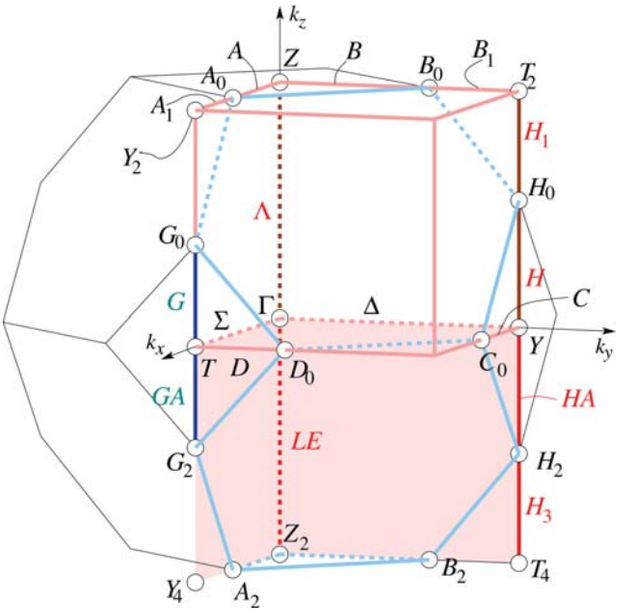


Fig. 1.5.5.5. Brillouin zone with asymmetric unit and representation domain of CDML for arithmetic crystal class *mm2F*: $a^{-2} < b^{-2} + c^{-2}$, $b^{-2} < c^{-2} + a^{-2}$ and $c^{-2} < a^{-2} + b^{-2}$. Space groups $Fmm2 - C_{2v}^{18}$ (42), $Fdd2 - C_{2v}^{19}$ (43). Reciprocal-space group $(Imm2)^*$, No. 44: $a^{*2} < b^{*2} + c^{*2}$, $b^{*2} < c^{*2} + a^{*2}$ and $c^{*2} < a^{*2} + b^{*2}$ (see Table 1.5.5.5). The representation domain of CDML is different from the asymmetric unit. Auxiliary points: T_4: $0, \frac{1}{2}, -\frac{1}{2}$; Y_2: $\frac{1}{2}, 0, \frac{1}{2}$; Y_4: $\frac{1}{2}, 0, -\frac{1}{2}$; Z_2: $0, 0, -\frac{1}{2}$. Flagpoles: $0, 0, z$: $-\frac{1}{2} < z < 0$; $0, \frac{1}{2}, z$: $-\frac{1}{2} < z < 0$. Wings: $x, 0, z$: $0 < x < \frac{1}{2}, -\frac{1}{2} < z < 0$; $0, y, z$: $0 < y < \frac{1}{2}, -\frac{1}{2} < z < 0$.

Table 1.5.5.5. *List of* ***k****-vector types for arithmetic crystal class mm2F:* $a^{-2} < b^{-2} + c^{-2}$, $b^{-2} < c^{-2} + a^{-2}$ *and* $c^{-2} < a^{-2} + b^{-2}$

See Fig. 1.5.5.5. Parameter relations: $x = -\frac{1}{2}\alpha + \frac{1}{2}\beta + \frac{1}{2}\gamma$, $y = \frac{1}{2}\alpha - \frac{1}{2}\beta + \frac{1}{2}\gamma$, $z = \frac{1}{2}\alpha + \frac{1}{2}\beta - \frac{1}{2}\gamma$.

k-vector label, CDML	Wyckoff position of *IT* A, *cf.* Section 1.5.4.3				Parameters
$\Gamma \quad 0, 0, 0$	*ex*	2	*a*	*mm2*	$0, 0, 0$
$Z \quad \frac{1}{2}, \frac{1}{2}, 0$	*ex*	2	*a*	*mm2*	$0, 0, \frac{1}{2}$
$\Lambda \quad \alpha, \alpha, 0$	*ex*	2	*a*	*mm2*	$0, 0, z$: $0 < z < \frac{1}{2}$
$LE \quad -\alpha, -\alpha, 0$	*ex*	2	*a*	*mm2*	$0, 0, z$: $-\frac{1}{2} < z < 0$
$\Gamma \cup \Lambda \cup Z \cup LE$		2	*a*	*mm2*	$0, 0, z$: $-\frac{1}{2} < z \leq \frac{1}{2}$
$T \quad 0, \frac{1}{2}, \frac{1}{2}$	*ex*	2	*b*	*mm2*	$\frac{1}{2}, 0, 0$
$T \sim T_2$					$0, \frac{1}{2}, \frac{1}{2}$
$Y \quad \frac{1}{2}, 0, \frac{1}{2}$	*ex*	2	*b*	*mm2*	$0, \frac{1}{2}, 0$
$G \quad \alpha, \frac{1}{2} + \alpha, \frac{1}{2}$	*ex*	2	*b*	*mm2*	$\frac{1}{2}, 0, z$: $0 < z \leq g_0$
$G \sim H_3 = [H_2\, T_4]$					$0, \frac{1}{2}, z$: $-\frac{1}{2} < z \leq -\frac{1}{2} + g_0 = h_2$
$GA \quad -\alpha, \frac{1}{2} - \alpha, \frac{1}{2}$	*ex*	2	*b*	*mm2*	$\frac{1}{2}, 0, z$: $g_2 = -g_0 < z < 0$
$GA \sim H_1 = [H_0\, T_2]$					$0, \frac{1}{2}, z$: $\frac{1}{2} - g_0 = h_0 < z < \frac{1}{2}$
$H \quad \frac{1}{2} + \alpha, \alpha, \frac{1}{2}$	*ex*	2	*b*	*mm2*	$0, \frac{1}{2}, z$: $0 < z \leq h_0$
$HA \quad \frac{1}{2} - \alpha, -\alpha, \frac{1}{2}$	*ex*	2	*b*	*mm2*	$0, \frac{1}{2}, z$: $h_2 = -h_0 < z < 0$
$T_2 \cup H_1 \cup H \cup Y \cup HA \cup H_3$		2	*b*	*mm2*	$0, \frac{1}{2}, z$: $-\frac{1}{2} < z \leq \frac{1}{2}$
$\Sigma \quad 0, \alpha, \alpha$	*ex*	4	*c*	*.m.*	$x, 0, 0$: $0 < x < \frac{1}{2}$
$A \quad \frac{1}{2}, \frac{1}{2} + \alpha, \alpha$	*ex*	4	*c*	*.m.*	$x, 0, \frac{1}{2}$: $0 < x \leq a_0$
$C \quad \frac{1}{2}, \alpha, \frac{1}{2} + \alpha$	*ex*	4	*c*	*.m.*	$x, \frac{1}{2}, 0$: $0 < x < c_0 = \frac{1}{2} - a_0$
$C \sim A_1$					$x, 0, \frac{1}{2}$: $\frac{1}{2} - a_0 = c_0 < x < \frac{1}{2}$
$J \quad \alpha, \alpha + \beta, \beta$	*ex*	4	*c*	*.m.*	$x, 0, z$: $[\Gamma\, Z\, A_0\, G_0\, T]$
$JA \quad -\alpha, -\alpha + \beta, \beta$	*ex*	4	*c*	*.m.*	$x, 0, z$: $[\Gamma\, T\, G_2\, A_2\, Z_2]$
$K \quad \frac{1}{2} + \alpha, \alpha + \beta, \frac{1}{2} + \beta$	*ex*	4	*c*	*.m.*	$x, \frac{1}{2}, z$: $[Y\, H_0\, C_0]$
$K \sim J_1$					$x, 0, z$: $[Y_4\, G_2\, A_2]$
$KA \quad \frac{1}{2} - \alpha, -\alpha + \beta, \frac{1}{2} + \beta$	*ex*	4	*c*	*.m.*	$x, \frac{1}{2}, z$: $[Y\, C_0\, H_2]$
$KA \sim J_3$					$x, 0, z$: $[Y_2\, G_0\, A_0]$
$A \cup A_1 \cup J \cup J_3 \cup \Sigma \cup JA \cup J_1$		4	*c*	*.m.*	$x, 0, z$: $0 < x < \frac{1}{2}$; $0 < z \leq \frac{1}{2}$
$\Delta \quad \alpha, 0, \alpha$	*ex*	4	*d*	*m..*	$0, y, 0$: $0 < y < \frac{1}{2}$
$B \quad \frac{1}{2} + \alpha, \frac{1}{2}, \alpha$	*ex*	4	*d*	*m..*	$0, y, \frac{1}{2}$: $0 < y < b_0$
$D \quad \alpha, \frac{1}{2}, \frac{1}{2} + \alpha$	*ex*	4	*d*	*m..*	$\frac{1}{2}, y, 0$: $0 < y \leq d_0$
$D \sim B_1$					$0, y, \frac{1}{2}$: $\frac{1}{2} - d_0 = b_0 \leq y < \frac{1}{2}$
$E \quad \alpha + \beta, \alpha, \beta$	*ex*	4	*d*	*m..*	$0, y, z$: $[\Gamma\, Y\, H_0\, B_0\, Z]$
$EA \quad -\alpha + \beta, -\alpha, \beta$	*ex*	4	*d*	*m..*	$0, y, z$: $[\Gamma\, Z_2\, B_2\, H_2\, Y]$
$F \quad \alpha + \beta, \frac{1}{2} + \alpha, \frac{1}{2} + \beta$	*ex*	4	*d*	*m..*	$\frac{1}{2}, y, z$: $[T\, D_0\, G_0]$
$F \sim E_3$					$0, y, z$: $[B_2\, T_4\, H_2]$
$FA \quad -\alpha + \beta, \frac{1}{2} - \alpha, \frac{1}{2} + \beta$	*ex*	4	*d*	*m..*	$\frac{1}{2}, y, z$: $[T\, G_2\, D_0]$
$FA \sim E_1$					$0, y, z$: $[T_2\, B_0\, H_0]$
$\Delta \cup B \cup B_1 \cup E \cup E_1 \cup EA \cup E_3$		4	*d*	*m..*	$0, y, z$: $0 < y < \frac{1}{2}$; $-\frac{1}{2} < z \leq \frac{1}{2}$
$GP \quad \alpha, \beta, \gamma$		8	*e*	1	x, y, z: $0 < x, y < \frac{1}{2}$; $0 < z \leq \frac{1}{2}$

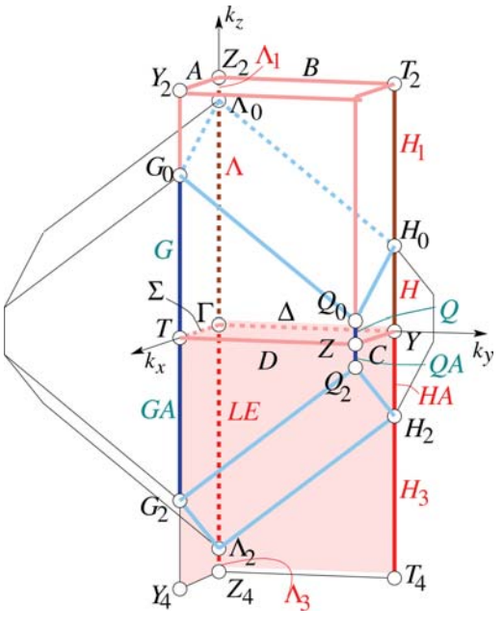


Fig. 1.5.5.6. Brillouin zone with asymmetric unit and representation domain of CDML for arithmetic crystal class *mm2F*: $c^{-2} > a^{-2} + b^{-2}$. Space groups $Fmm2 - C_{2v}^{18}$ (42), $Fdd2 - C_{2v}^{19}$ (43). Reciprocal-space group (*Imm2*)*, No. 44: $c^{*2} > a^{*2} + b^{*2}$ (see Table 1.5.5.6). The representation domain of CDML is different from the asymmetric unit. Auxiliary points: T_4: $0, \frac{1}{2}, -\frac{1}{2}$; Y_4: $\frac{1}{2}, 0, -\frac{1}{2}$; Z_4: $0, 0, -\frac{1}{2}$. Flagpoles: $0, 0, z$: $-\frac{1}{2} < z < 0$; $0, \frac{1}{2}, z$: $-\frac{1}{2} < z < 0$. Wings: $x, 0, z$: $0 < x < \frac{1}{2}, -\frac{1}{2} < z < 0$; $0, y, z$: $0 < y < \frac{1}{2}, -\frac{1}{2} < z < 0$.

Table 1.5.5.6. *List of* **k***-vector types for arithmetic crystal class mm2F:* $c^{-2} > a^{-2} + b^{-2}$

See Fig. 1.5.5.6. Parameter relations: $x = -\frac{1}{2}\alpha + \frac{1}{2}\beta + \frac{1}{2}\gamma$, $y = \frac{1}{2}\alpha - \frac{1}{2}\beta + \frac{1}{2}\gamma$, $z = \frac{1}{2}\alpha + \frac{1}{2}\beta - \frac{1}{2}\gamma$.

k-vector label, CDML	Wyckoff position of *IT* A, *cf.* Section 1.5.4.3	Parameters
Γ $0, 0, 0$	*ex* 2 *a* *mm2*	$0, 0, 0$
Z $\frac{1}{2}, \frac{1}{2}, 1$	*ex* 2 *a* *mm2*	$\frac{1}{2}, \frac{1}{2}, 0$
$Z \sim Z_2$		$0, 0, \frac{1}{2}$
Λ $\alpha, \alpha, 0$	*ex* 2 *a* *mm2*	$0, 0, z$: $0 < z \le \lambda_0$
LE $-\alpha, -\alpha, 0$	*ex* 2 *a* *mm2*	$0, 0, z$: $\lambda_2 = -\lambda_0 < z < 0$
Q $\frac{1}{2}+\alpha, \frac{1}{2}+\alpha, 1$	*ex* 2 *a* *mm2*	$\frac{1}{2}, \frac{1}{2}, z$: $0 < z \le q_0$
$Q \sim \Lambda_3 = [\Lambda_2\, Z_4]$		$0, 0, z$: $-\frac{1}{2} < z \le -\frac{1}{2} + q_0 = -\lambda_0$
QA $\frac{1}{2}-\alpha, \frac{1}{2}-\alpha, 1$	*ex* 2 *a* *mm2*	$\frac{1}{2}, \frac{1}{2}, z$: $q_2 = -q_0 < z < 0$
$QA \sim \Lambda_1 = [\Lambda_0\, Z_2]$		$0, 0, z$: $\frac{1}{2} - q_0 = \lambda_0 < z < \frac{1}{2}$
$Z_2 \cup \Lambda_1 \cup \Lambda \cup \Gamma \cup LE \cup \Lambda_3$	2 *a* *mm2*	$0, 0, z$: $-\frac{1}{2} < z \le \frac{1}{2}$
T $0, \frac{1}{2}, \frac{1}{2}$	*ex* 2 *b* *mm2*	$\frac{1}{2}, 0, 0$
$T \sim T_2$		$0, \frac{1}{2}, \frac{1}{2}$
Y $\frac{1}{2}, 0, \frac{1}{2}$	*ex* 2 *b* *mm2*	$0, \frac{1}{2}, 0$
G $\alpha, \frac{1}{2}+\alpha, \frac{1}{2}$	*ex* 2 *b* *mm2*	$\frac{1}{2}, 0, z$: $0 < z \le g_0$
$G \sim H_3 = [H_2\, T_4]$		$0, \frac{1}{2}, z$: $-\frac{1}{2} < z \le -\frac{1}{2} + g_0$
GA $-\alpha, \frac{1}{2}-\alpha, \frac{1}{2}$	*ex* 2 *b* *mm2*	$\frac{1}{2}, 0, z$: $g_2 = -g_0 < z < 0$
$GA \sim H_1 = [H_0\, T_2]$		$0, \frac{1}{2}, z$: $\frac{1}{2} - g_0 = h_0 < z < \frac{1}{2}$
H $\frac{1}{2}+\alpha, \alpha, \frac{1}{2}$	*ex* 2 *b* *mm2*	$0, \frac{1}{2}, z$: $0 < z \le h_0$
HA $\frac{1}{2}-\alpha, -\alpha, \frac{1}{2}$	*ex* 2 *b* *mm2*	$0, \frac{1}{2}, z$: $h_2 = -h_0 < z < 0$
$T_2 \cup H_1 \cup H \cup Y \cup HA \cup H_3$	2 *b* *mm2*	$0, \frac{1}{2}, z$: $-\frac{1}{2} < z \le \frac{1}{2}$
Σ $0, \alpha, \alpha$	*ex* 4 *c* *.m.*	$x, 0, 0$: $0 < x < \frac{1}{2}$
C $\frac{1}{2}, \alpha, \frac{1}{2}+\alpha$	*ex* 4 *c* *.m.*	$x, \frac{1}{2}, 0$: $0 < x < \frac{1}{2}$
$C \sim A = [Z_2\, Y_2]$		$x, 0, \frac{1}{2}$: $0 < z < \frac{1}{2}$
J $\alpha, \alpha+\beta, \beta$	*ex* 4 *c* *.m.*	$x, 0, z$: $[\Gamma\, \Lambda_0\, G_0\, T]$
JA $-\alpha, -\alpha+\beta, \beta$	*ex* 4 *c* *.m.*	$x, 0, z$: $[\Gamma\, T\, G_2\, \Lambda_2]$
K $\frac{1}{2}+\alpha, \alpha+\beta, \frac{1}{2}+\beta$	*ex* 4 *c* *.m.*	$x, \frac{1}{2}, z$: $[Y\, H_0\, Q_0\, Z]$
$K \sim J_3$		$x, 0, z$: $[Y_4\, G_2\, \Lambda_2\, Z_4]$
KA $\frac{1}{2}-\alpha, -\alpha+\beta, \frac{1}{2}+\beta$	*ex* 4 *c* *.m.*	$x, \frac{1}{2}, z$: $[Z\, Q_2\, H_2\, Y]$
$KA \sim J_1$		$x, 0, z$: $[Z_2\, Y_2\, G_0\, \Lambda_0]$
$A \cup J_1 \cup J \cup \Sigma \cup JA \cup J_3$	4 *c* *.m.*	$x, 0, z$: $0 < x < \frac{1}{2}$; $-\frac{1}{2} < z \le \frac{1}{2}$
Δ $\alpha, 0, \alpha$	*ex* 4 *d* *m..*	$0, y, 0$: $0 < y < \frac{1}{2}$
D $\alpha, \frac{1}{2}, \frac{1}{2}+\alpha$	*ex* 4 *d* *m..*	$\frac{1}{2}, y, 0$: $0 < y < \frac{1}{2}$
$D \sim B$		$0, y, \frac{1}{2}$: $0 < y < \frac{1}{2}$
E $\alpha+\beta, \alpha, \beta$	*ex* 4 *d* *m..*	$0, y, z$: $[\Gamma\, Y\, H_0\, \Lambda_0]$
EA $-\alpha+\beta, -\alpha, \beta$	*ex* 4 *d* *m..*	$0, y, z$: $[\Gamma\, \Lambda_2\, H_2\, Y]$
F $\alpha+\beta, \frac{1}{2}+\alpha, \frac{1}{2}+\beta$	*ex* 4 *d* *m..*	$\frac{1}{2}, y, z$: $[T\, Z\, Q_0\, G_0]$
$F \sim E_3$		$0, y, z$: $[Z_4\, \Lambda_2\, H_2\, T_4]$
FA $-\alpha+\beta, \frac{1}{2}-\alpha, \frac{1}{2}+\beta$	*ex* 4 *d* *m..*	$\frac{1}{2}, y, z$: $[T\, G_2\, Q_2\, Z]$
$FA \sim E_1$		$0, y, z$: $[Z_2\, \Lambda_0\, H_0\, T_2]$
$B \cup E_1 \cup E \cup \Delta \cup EA \cup E_3$	4 *d* *m..*	$0, y, z$: $0 < y < \frac{1}{2}$; $-\frac{1}{2} < z \le \frac{1}{2}$
GP α, β, γ	8 *e* 1	x, y, z: $0 < x, y < \frac{1}{2}$; $0 < z \le \frac{1}{2}$

In general the sequence of the Wyckoff letters in *IT* A follows the falling number of free parameters. In the few cases where the sequence in *IT* A is different, the Wyckoff letters are exchanged. The exchange is noted at the top of the table.

Example. In the arithmetic crystal class $4/mmmI$, $c/a < 1$, see Table 1.5.5.3, Wyckoff position *e* has one free parameter, whereas Wyckoff position *f* has constant parameters, *i.e.* no free parameter. Therefore, *f* is listed above the horizontal line, *e* is listed below, see Table 1.5.5.3. The note at the top of the table states 'Wyckoff positions *e* and *f* exchanged'.

Parameter relations. The relations between the parameters of CDML and the parameters referred to the asymmetric unit are listed at the top of the table, *e.g.* for $m\bar{3}mI$ in Table 1.5.5.1: 'Parameter relations: $x = \frac{1}{2}\beta + \frac{1}{2}\gamma$, $y = \frac{1}{2}\alpha + \frac{1}{2}\gamma$, $z = \frac{1}{2}\alpha + \frac{1}{2}\beta$'. These relations may be modified to more convenient parameters without notice, as for the plane *B* of $m\bar{3}mI$ in Table 1.5.5.1:

$$B \quad \alpha+\beta, -\alpha+\beta, \tfrac{1}{2}-\beta \quad ex\ 96\ k\ ..m \quad x, \tfrac{1}{2}-x, z\colon\ 0 < z < x < \tfrac{1}{4}$$

instead of

$$\ldots \tfrac{1}{4} - \tfrac{1}{2}\alpha, \tfrac{1}{4} + \tfrac{1}{2}\alpha, \beta\colon\ 0 < \alpha < \tfrac{1}{2} - 2\beta < \tfrac{1}{2}.$$

1.5.5.3. Figures and tables

Arithmetic crystal classes $m\bar{3}mI$ *and* $m\bar{3}I$: The reciprocal lattice of a cubic lattice *I* is a cubic lattice *F*. Its Brillouin zone is a rhombic dodecahedron and has 12 faces, 24 edges and 14 apices, the coordinates of which are the six permutations of $\pm\frac{1}{2}, 0, 0$ and the eight coordinate triplets of $\pm\frac{1}{4}, \pm\frac{1}{4}, \pm\frac{1}{4}$. Eleven of these 14 points are visible in the applied projection.

The figure for arithmetic crystal class $m\bar{3}mI$ is shown in Fig. 1.5.5.1 and the corresponding table is Table 1.5.5.1. The figure for arithmetic crystal class $m\bar{3}I$ is shown in Fig. 1.5.5.2 and the corresponding table is Table 1.5.5.2.

Arithmetic crystal class $4/mmmI$: There are two different types of Brillouin zones for the tetragonal *I* lattice, one for $c < a$ (Fig. 1.5.5.3, Table 1.5.5.3) and one for $c > a$ (Fig. 1.5.5.4, Table 1.5.5.4). The first type of Brillouin zone, Fig. 1.5.5.3, is a tetragonal elongated rhombdodecahedron with 12 faces, four of them being hexagons. There are 18 apices; 14 of them are visible. The Brillouin zone of Fig. 1.5.5.4 is a tetragonally deformed cuboctahedron with 14 faces. There are 24 apices; 18 of them are visible.

Arithmetic crystal class mm2F: Depending on the lattice ratios *a*:*b*:*c*, there are four figures in CDML for the Brillouin zone of an orthorhombic crystal with an *F* lattice, see Fig. 3.6 on p. 26 in CDML. Only three of them are really necessary. Therefore, the case $b^{-2} > c^{-2} + a^{-2}$ of Fig. 3.6(c) of CDML has been omitted in these examples; it is obtained from $a^{-2} > c^{-2} + b^{-2}$ of Figure 3.6(d) by a rotation by 90° about the *c** axis. The three remaining

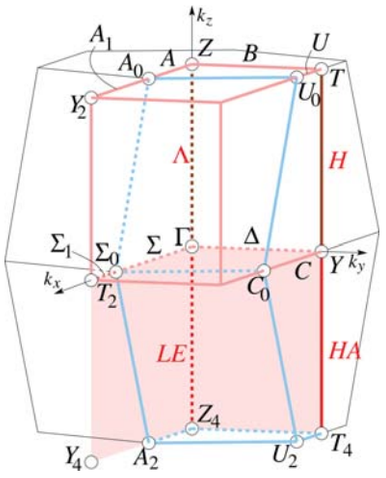


Fig. 1.5.5.7. Brillouin zone with asymmetric unit and representation domain of CDML for arithmetic crystal class *mm2F*: $a^{-2} > b^{-2} + c^{-2}$. Space groups $Fmm2 - C_{2v}^{18}$ (42), $Fdd2 - C_{2v}^{19}$ (43). Reciprocal-space group $(Imm2)^*$, No. 44: $a^{*2} > b^{*2} + c^{*2}$ (see Table 1.5.5.7). The representation domain of CDML is different from the asymmetric unit. Auxiliary points: T_4: $0, \frac{1}{2}, -\frac{1}{2}$; Y_4: $\frac{1}{2}, 0, -\frac{1}{2}$; Z_4: $0, 0, -\frac{1}{2}$. Flagpoles: $LE = [Z_4\,\Gamma]$ $0, 0, z$: $-\frac{1}{2} < z < 0$; $HA = [T_4\,Y]$ $0, \frac{1}{2}, z$: $-\frac{1}{2} < z < 0$. Wings: $JA \cup J_3 = [\Gamma\,T_2\,Y_4\,Z_4]$ $x, 0, z$: $0 < x < \frac{1}{2}, -\frac{1}{2} < z < 0$; $EA = [\Gamma\,Z_4\,T_4\,Y]$ $0, y, z$: $0 < y < \frac{1}{2}, -\frac{1}{2} < z < 0$.

Brillouin zones are displayed in Fig. 1.5.5.5 (see also Table 1.5.5.5), Fig. 1.5.5.6 (see also Table 1.5.5.6) and Fig. 1.5.5.7 (see also Table 1.5.5.7). Fig. 1.5.5.5 is a distorted cuboctahedron with 14 faces, 36 edges and 24 apices, 18 of which are visible. The Brillouin zones of Figs. 1.5.5.6 and 1.5.5.7 are distorted elongated rhombdodecahedra. There are 12 faces, 28 edges and 18 apices; 14 of them are visible.

1.5.5.4. Discussion

1.5.5.4.1. Representation domains and asymmetric units

When the symmetry of the reciprocal lattice allows, the shape of the asymmetric unit may be chosen to be much simpler than that of the representation domain.

Examples

(1) Arithmetic crystal class $4/mmmI$. The parameter ranges for the special lines and planes of the asymmetric unit and for general **k** vectors of the reciprocal-space group $(F4/mmm)^*$ [setting $(I4/mmm)^*$] are listed in Tables 1.5.5.3 and 1.5.5.4. One can describe the corresponding conditions of the representation domain by the boundary plane $x, y, z = \{1 + (c/a)^2[1 - 2(x + y)]\}/4$ which for $c/a < 1$ forms the triangle $[Z_0\,Z_2\,P]$ in Fig. 1.5.5.3 but for $c/a > 1$ the pentagon $[S_2\,R\,P\,G\,S]$ in Fig. 1.5.5.4. The inner points of this boundary plane 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, $x, y, z = \frac{1}{4}$, for the asymmetric unit.

(2) Arithmetic crystal class *mm2F*, see Figs. 1.5.5.5 to 1.5.5.7. In the reciprocal-space group $(Imm2)^*$ the lines Λ and *LE* belong to Wintgen position 2 *a mm*2, as do the lines *Q*, *QA*, Λ_1 and Λ_3 if present. The lines *H* and *HA* belong to the Wintgen position 2 *b mm*2; as do the lines *G*, *GA*, H_1 and H_3 if present. The lines Σ, Σ_1, *A*, A_1, *C* and *U* belong to the plane $x, 0, z$; the lines Δ, *B*, B_1 and *D* belong to the plane $0, y, z$. The decisive boundary plane of the representation domain is $xa^{*2} + yb^{*2} + zc^{*2} = d^{*2}/4$, where $d^{*2} = a^{*2} + b^{*2} + c^{*2}$; it is a hexagon for Fig. 1.5.5.5 and a parallelogram for Figs. 1.5.5.6 and 1.5.5.7. There is no relation of the lattice parameters for which all the above-mentioned lines are realized on the surface of the representation domain simultaneously; either two or

Table 1.5.5.7. *List of* **k***-vector types for arithmetic crystal class mm2F:* $a^{-2} > b^{-2} + c^{-2}$

See Fig. 1.5.5.7. Parameter relations: $x = -\frac{1}{2}\alpha + \frac{1}{2}\beta + \frac{1}{2}\gamma$, $y = \frac{1}{2}\alpha - \frac{1}{2}\beta + \frac{1}{2}\gamma$, $z = \frac{1}{2}\alpha + \frac{1}{2}\beta - \frac{1}{2}\gamma$.

k-vector label, CDML	Wyckoff position of *IT* A, *cf.* Section 1.5.4.3				Parameters
Γ $0, 0, 0$	*ex*	2	*a*	*mm2*	$0, 0, 0$
Z $\frac{1}{2}, \frac{1}{2}, 0$	*ex*	2	*a*	*mm2*	$0, 0, \frac{1}{2}$
Λ $\alpha, \alpha, 0$	*ex*	2	*a*	*mm2*	$0, 0, z$: $0 < z < \frac{1}{2}$
LE $-\alpha, -\alpha, 0$	*ex*	2	*a*	*mm2*	$0, 0, z$: $-\frac{1}{2} < z < 0$
$\Gamma \cup Z \cup \Lambda \cup LE$		2	*a*	*mm2*	$0, 0, z$: $-\frac{1}{2} < z \leq \frac{1}{2}$
T $1, \frac{1}{2}, \frac{1}{2}$	*ex*	2	*b*	*mm2*	$0, \frac{1}{2}, \frac{1}{2}$
Y $\frac{1}{2}, 0, \frac{1}{2}$	*ex*	2	*b*	*mm2*	$0, \frac{1}{2}, 0$
H $\frac{1}{2} + \alpha, \alpha, \frac{1}{2}$	*ex*	2	*b*	*mm2*	$0, \frac{1}{2}, z$: $0 < z < \frac{1}{2}$
HA $\frac{1}{2} - \alpha, -\alpha, \frac{1}{2}$	*ex*	2	*b*	*mm2*	$0, \frac{1}{2}, z$: $-\frac{1}{2} < z < 0$
$T \cup Y \cup H \cup HA$		2	*b*	*mm2*	$0, \frac{1}{2}, z$: $-\frac{1}{2} < z \leq \frac{1}{2}$
Σ $0, \alpha, \alpha$	*ex*	4	*c*	*.m.*	$x, 0, 0$: $0 < x \leq \sigma_0$
U $1, \frac{1}{2} + \alpha, \frac{1}{2} + \alpha$	*ex*	4	*c*	*.m.*	$x, \frac{1}{2}, \frac{1}{2}$: $0 < x < u_0$
$U \sim \Sigma_1 = [\Sigma_0\,T_2]$					$x, 0, 0$: $\frac{1}{2} - u_0 = \sigma_0 < x < \frac{1}{2}$
A $\frac{1}{2}, \frac{1}{2} + \alpha, \alpha$	*ex*	4	*c*	*.m.*	$x, 0, \frac{1}{2}$: $0 < x < a_0$
C $\frac{1}{2}, \alpha, \frac{1}{2} + \alpha$	*ex*	4	*c*	*.m.*	$x, \frac{1}{2}, 0$: $0 < x \leq c_0$
$C \sim A_1 = [A_0\,Y_2]$					$x, 0, \frac{1}{2}$: $a_0 = \frac{1}{2} - c_0 \leq x < \frac{1}{2}$
J $\alpha, \alpha + \beta, \beta$	*ex*	4	*c*	*.m.*	$x, 0, z$: $[\Gamma\,Z\,A_0\,\Sigma_0]$
JA $-\alpha, -\alpha + \beta, \beta$	*ex*	4	*c*	*.m.*	$x, 0, z$: $[\Gamma\,\Sigma_0\,A_2\,Z_4]$
K $\frac{1}{2} + \alpha, \alpha + \beta, \frac{1}{2} + \beta$	*ex*	4	*c*	*.m.*	$x, \frac{1}{2}, z$: $[Y\,T\,U_0\,C_0]$
$K \sim J_3$					$x, 0, z$: $[T_2\,\Sigma_0\,A_2\,Y_4]$
KA $\frac{1}{2} - \alpha, -\alpha + \beta, \frac{1}{2} + \beta$	*ex*	4	*c*	*.m.*	$x, \frac{1}{2}, z$: $[Y\,C_0\,U_2\,T_4]$
$KA \sim J_1$					$x, 0, z$: $[T_2\,\Sigma_0\,A_0\,Y_2]$
$A \cup A_1 \cup J \cup J_1 \cup \Sigma \cup \Sigma_1 \cup JA \cup J_3$		4	*c*	*.m.*	$x, 0, z$: $0 < x < \frac{1}{2}, -\frac{1}{2} < z \leq \frac{1}{2}$
Δ $\alpha, 0, \alpha$	*ex*	4	*d*	*m..*	$0, y, 0$: $0 < y < \frac{1}{2}$
B $\frac{1}{2} + \alpha, \frac{1}{2}, \alpha$	*ex*	4	*d*	*m..*	$0, y, \frac{1}{2}$: $0 < y < \frac{1}{2}$
E $\alpha + \beta, \alpha, \beta$	*ex*	4	*d*	*m..*	$0, y, z$: $0 < y, z < \frac{1}{2}$
EA $-\alpha + \beta, -\alpha, \beta$	*ex*	4	*d*	*m..*	$0, y, z$: $0 < y < \frac{1}{2}, -\frac{1}{2} < z < 0$
$\Delta \cup B \cup E \cup EA$		4	*d*	*m..*	$0, y, z$: $0 < y < \frac{1}{2}, -\frac{1}{2} < z \leq \frac{1}{2}$
GP α, β, γ		8	*e*	1	x, y, z: $0 < x, y < \frac{1}{2}, 0 \leq z < \frac{1}{2}$

three of them do not appear and the length of the others depends on the boundary plane, see Tables and Figs. 1.5.5.5 to 1.5.5.7.

The boundary conditions for the asymmetric unit are independent of the lattice parameters and the boundary plane is always represented by the simple equation $x, y, \frac{1}{2}$: $0 < x, y < \frac{1}{2}$. By introducing flagpoles and wings, the description may become uni-arm.

1.5.5.4.2. Splitting of **k**-vector types

The Brillouin zone as well as the unit cell are always convex bodies; the same holds for the representation domain of CDML and for the choice of the asymmetric unit. It is thus sometimes unavoidable that the **k**-vector types are split and that the different parts belong to different arms and to different stars of **k** vectors. Sometimes this splitting of **k**-vector types may be avoided by an appropriate choice of the asymmetric unit; sometimes the introduction of flagpoles and wings is necessary to make the **k**-vector types uni-arm.

Examples

(1) In the reciprocal-space group $(\mathcal{G})^* = (Fm\bar{3}m)^*$, No. 225 of the arithmetic crystal class $m\bar{3}mI$ there are the lines of **k** vectors Λ (α, α, α) and F $(\frac{1}{2} - \alpha, -\frac{1}{2} + 3\alpha, \frac{1}{2} - \alpha)$ of CDML, p. 41. By Figure 1.5.5.1 one sees that the line Λ connects the points Γ and P, the line F connects the points P and H. One takes from the corresponding Table 1.5.5.1 the coefficients of $P = \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ and $H = 0, \frac{1}{2}, 0$. From these points or from the transformation listed at the top of Table 1.5.5.1 as 'Parameter relations' the coefficients of the line F are obtained as $F = x, \frac{1}{2} - x, x$; $0 < x < \frac{1}{4}$.

The inspection of the symmetry diagram of $Fm\bar{3}m$, No. 225, in *IT* A shows that a twofold rotation 2 (represented by the 4_2 $\frac{1}{4}, y, \frac{1}{4}$ screw-rotation axis) leaves the point P invariant, whereas the point H is mapped onto the point R $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$. More formally: the rotation is described by $x, \frac{1}{2} - x, x \rightarrow \frac{1}{2} - x, \frac{1}{2} - x, \frac{1}{2} - x$, where $0 < x < \frac{1}{4}$. The result is the line $F_1 = [R\,P]$. It is uni-arm to the line $\Lambda = x, x, x$ and the union $\Lambda \cup F_1$ forms the Wintgen position 32 *f* 3*m*. An analoguous result is obtained for the same lines in the arithmetic crystal class $m\bar{3}I$.

(2) In the following example the splitting of a Wintgen position happens if a representation domain of the Brillouin zone is chosen. The splitting can be avoided by the choice of the asymmetric unit. We consider the plane $x, y, 0$ in the arithmetic crystal class $4/mmmI$, see Fig. 1.5.5.4 and Table 1.5.5.4. In CDML this plane is split into the parts $C = [\Gamma\,S_2\,R\,X]$ and $D = [M\,S\,G] \sim [M_2\,S_2\,R]$. By the choice of the asymmetric unit the independent region of the Wintgen position is uni-arm: $[\Gamma M_2 X] = 16\ l\ m..\ x, y, 0$: $0 < x < y < \frac{1}{2}$.

(3) The splitting of a Wintgen position can be avoided if flagpoles and wings are admitted, *i.e.* if the minimal domain is described by a non-convex body. If one chooses in the first example of the arithmetic crystal classes $m\bar{3}mI$ and $m\bar{3}I$ the union $\Lambda \cup F_1$ for the line x, x, x, then $F_1 = [P\,R]$ forms a flagpole, whereas Λ forms an edge of the asymmetric unit, see Figs. 1.5.5.1 and 1.5.5.2.

The same holds for the Wintgen position 96 *k* ..*m* x, x, z of $m\bar{3}mI$. In the representation domain which is simultaneously the asymmetric unit, this Wintgen position is split into three parts *B*, *C* and *J*, which form three of the four walls of the (tetrahedral) minimal domain. By proper symmetry operations these three parts can be made uni-arm to the part *C*, such that their union $C \cup B_1 \cup J_1$ describes the independent part of that Wintgen position, see Fig. 1.5.5.1. The part *C* forms a wall of the asymmetric unit; the part $B_1 \cup J_1$ forms a wing, see Fig. 1.5.5.1.

1.5.5.4.3. **k**-vector types for non-holosymmetric space groups

The **k**-vector labels of CDML are primarily listed for the holosymmetric space groups. These lists are kept and supplemented for the non-holosymmetric space groups. In this way many superfluous **k**-vector labels are introduced.

Examples

(1) Arithmetic crystal class $m\bar{3}I$. In its reciprocal-space group $(Fm\bar{3})^*$, the introduction of the plane $AA = [\Gamma\,H_2\,N]$ is unnecessary because the plane $A = [\Gamma\,N\,H]$ of Wintgen position 96 *j* *m*.. of $(Fm\bar{3}m)^*$ can be extended to $A \cup AA = [\Gamma\,H_2\,H]$ in the reciprocal-space group $(Fm\bar{3})^*$, *cf.* Fig. 1.5.5.2 and Table 1.5.5.2. In $(Fm\bar{3})^*$, both planes, *A* and *AA*, belong to Wintgen position 48 *h* *m*... The parameter description is extended from $x, y, 0$: $0 < x < y < \frac{1}{2} - x (< \frac{1}{4})$ to $0 < y < \frac{1}{2} - x < \frac{1}{2}$.

(2) In the previous example, during the transition from the group $(Fm\bar{3}m)^*$ to the subgroup $(Fm\bar{3})^*$ the order of the little co-group of the special **k** vectors of $(Fm\bar{3}m)^*$ was not changed. In other cases, the little co-group may be reduced to a subgroup. Such **k** vectors may then be incorporated into a more general Wintgen position and described by an extension of the parameter range.

Arithmetic crystal class $m\bar{3}mI$, plane $[\Gamma\,H\,N] = x, y, 0$. In $(Fm\bar{3}m)^*$, see Fig. 1.5.5.1, all points (Γ, H, N) and lines (Δ, Σ, G) of the boundary of the asymmetric unit are special. In $(Fm\bar{3})^*$, see Fig. 1.5.5.2, the lines Δ and $[\Gamma\,H_2] \sim \Delta$ are special but Σ, *G* and $[N\,H_2] \sim G$ belong to the plane $(A \cup AA)$. The free parameter range on the line *G* is $0 < y < \frac{1}{4}$. Therefore, the parameter ranges of $(A \cup AA \cup G \cup \Sigma)$ in $x, y, 0$ can be taken as: $0 < x < \frac{1}{2} - y < \frac{1}{2}$ for $A \cup AA \cup \Sigma$ and $0 < y = \frac{1}{2} - x < \frac{1}{4}$ for *G*.

1.5.5.4.4. Ranges of independent parameters

In Section 1.5.4.3 a method for the determination of the parameter ranges was described. A few examples shall display the procedure.

(1) Arithmetic crystal class $m\bar{3}mI$, line $\Lambda \cup F_1$: In the reciprocal-space group $(Fm\bar{3}m)^*$ of the arithmetic crystal class $m\bar{3}mI$, the line x, x, x has stabilizer $\bar{3}m$ and little co-group $\overline{\mathcal{G}}^{\mathbf{k}} = 3m$. Therefore, the divisor is 12:6 = 2 and x is running from 0 to $\frac{1}{2}$.

The same result holds for the line $\Lambda \cup F_1$ in the reciprocal-space group $(Fm\bar{3})^*$ of the arithmetic crystal class $m\bar{3}I$: the stabilizer generated by $\bar{3}$ is of order 6, $|\overline{\mathcal{G}}^{\mathbf{k}}| = |\{\bar{3}\}| = 3$, the quotient is again $\frac{1}{2}$, the parameter range is the same as for $(Fm\bar{3}m)^*$.

(2) Arithmetic crystal class $m\bar{3}mI$, plane $B_1 \cup C \cup J_1$: In $(Fm\bar{3}m)^*$, the stabilizer of x, x, z is generated by *m*.*mm* and the centring translation $t(\frac{1}{2}, \frac{1}{2}, 0)$ mod (integer translations). They generate a group of order 16; $\overline{\mathcal{G}}^{\mathbf{k}}$ is ..*m* of order 2. The fraction of the plane is $\frac{2}{16} = \frac{1}{8}$ of the area $\sqrt{2}a^{*2}$ in the (centred) unit cell, 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 (x, x, z, $\bar{x}, x, z$ and x, y, x) are represented in the boundaries of the representation domain: $C = [\Gamma\,N\,P]$, $B = [H\,N\,P]$ and $J = [\Gamma\,H\,P]$, 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 $\frac{1}{8}$.

Arithmetic crystal class $m\bar{3}I$, the same result holds in the reciprocal-space group $(Fm\bar{3})^*$. The stabilizer generated by $2/m$.. and by the centring translation $t(\frac{1}{2}, \frac{1}{2}, 0)$ mod (integer translations) forms a group of order 8; the order of the little co-group $|\overline{\mathcal{G}}^{\mathbf{k}}| = |\{1\}| = 1$. The quotient is again $\frac{1}{8}$, the parameter range is the same as for $(Fm\bar{3}m)^*$ but the plane belongs to the general position *GP* because the little co-group is trivial.

(3) Arithmetic crystal class $m\bar{3}mI$, reciprocal-space group $(Fm\bar{3}m)^*$, plane $x, y, 0$: the stabilizer of the plane *A* is generated by $4/mmm$ and $t(\frac{1}{2}, \frac{1}{2}, 0)$, order 32, $\overline{\mathcal{G}}^{\mathbf{k}}$ (site-symmetry group) *m*..,

order 2. Consequently, $[\Gamma\ H\ N]$ is $\frac{1}{16}$ of the unit square a^{*2}: $0 < x < y < \frac{1}{2} - x$. In $(Fm\overline{3})^*$, the stabilizer of $x, y, 0$, here $A \cup AA$, is mmm. and $t(\frac{1}{2}, \frac{1}{2}, 0)$, order 16, with the same group $\overline{\mathcal{G}}^{\mathbf{k}} = m..$ of order 2. Therefore, $[\Gamma\ H_2\ H]$ is $\frac{1}{8}$ of the unit square a^{*2} in $(Fm\overline{3})^*$; $0 < y < \frac{1}{2} - x < \frac{1}{2}$.

(4) Arithmetic crystal class $m\overline{3}mI$, line $x, x, 0$: In $(Fm\overline{3}m)^*$ the stabilizer is generated by $m.mm$ and $t(\frac{1}{2}, \frac{1}{2}, 0)$ mod (integer translations), order 16, $\overline{\mathcal{G}}^{\mathbf{k}}$ is $m.2m$ of order 4. The divisor is 4 and thus $0 < x < \frac{1}{4}$. In $(Fm\overline{3})^*$ the stabilizer is generated by $2/m..$ and $t(\frac{1}{2}, \frac{1}{2}, 0)$ mod (integer translations), order 8, and $\overline{\mathcal{G}}^{\mathbf{k}} = m..$, order 2; the divisor is 4 again and $0 < x < \frac{1}{4}$ is restricted to the same range.

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

(1) Arithmetic crystal classes $m\overline{3}mI$ and $m\overline{3}I$, *i.e.* $(Fm\overline{3}m)^*$ and $(Fm\overline{3})^*$, line x, x, x: 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: $0 < x < \frac{1}{4}$, $\frac{1}{4} < x < \frac{1}{2}$.

(2) Arithmetic crystal class $m\overline{3}mI$, plane x, x, z: In $(Fm\overline{3}m)^*$ all corners Γ, N, N_2, H_2 and all edges are special points or 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: $0 < x < \frac{1}{4}$ and $x, x, \frac{1}{2} - x$: $0 < x < \frac{1}{4}$ are special lines and thus excepted.

(3) Arithmetic crystal classes $m\overline{3}mI$ and $m\overline{3}I$, plane $x, y, 0$: In both reciprocal-space groups, $(Fm\overline{3}m)^*$ and $(Fm\overline{3})^*$, $0 < x$ and $0 < y$ holds. The line $0, y, 0 = \Delta$ is a special line, its $\mathbf{k}$ vectors have little co-groups of higher order than that of the planes $x, y, 0$ and the boundaries of both planes are open. The same holds for the boundary $x, 0, 0 \sim 0, y, 0$ for $(Fm\overline{3})^*$. The $\mathbf{k}$ vectors of the lines $x, x, 0$ and $x, \frac{1}{2} - x, 0$, Σ and G, also have little co-groups of higher order and belong to other Wintgen positions in the representation domain (or asymmetric unit) of $(Fm\overline{3}m)^*$. Therefore, for the arithmetic crystal class $m\overline{3}mI$, the plane $A = x, y, 0$ is open at its boundaries $x, x, 0$ and $x, \frac{1}{2} - x, 0$ in the range $0 < x < \frac{1}{4}$. In the asymmetric unit of $(Fm\overline{3})^*$ the lines $x, x, 0$: $0 < x < \frac{1}{4}$ and $x, \frac{1}{2} - x, 0$: $0 < x < \frac{1}{4}$ belong to the plane, and the boundary of the plane A is here closed. The boundary line $x, \frac{1}{2} - x, 0$: $\frac{1}{4} < x < \frac{1}{2}$ of the plane AA is equivalent to the range $0 < x < \frac{1}{4}$ of the part A and thus does not belong to the asymmetric unit; here the boundary of the plane $A \cup AA$ is open.

1.5.6. Conclusions

International Tables for Crystallography Volume A can serve as a basis for the classification of irreps of space groups by using the concept of reciprocal-space groups. The main features of the crystallographic classification scheme are as follows.

(i) The asymmetric units of the conventional crystallographic unit cells are minimal domains of $\mathbf{k}$ space which are in many cases simpler than the representation domains of the Brillouin zones.

(ii) All $\mathbf{k}$-vector stars giving rise to the same type of irreps belong to the same Wintgen position and *vice versa*. They can be collected in one entry (uni-arm description) and are designated by the same Wintgen letter if flagpoles and wings are admitted.

(iii) The Wyckoff positions of *IT* A, interpreted as Wintgen positions, provide a complete list of the special $\mathbf{k}$ vectors in the Brillouin zone; the site symmetry of *IT* A is the little co-group $\overline{\mathcal{G}}^{\mathbf{k}}$ of $\mathbf{k}$; the multiplicity per primitive unit cell is the number of arms of the star of $\mathbf{k}$. The Wintgen positions with 0, 1, 2, or 3 variable parameters correspond to special $\mathbf{k}$-vector points, $\mathbf{k}$-vector lines, $\mathbf{k}$-vector planes or to the set of all general $\mathbf{k}$ vectors, respectively.

The complete set of types of irreps is obtained by considering the irreps of one $\mathbf{k}$ vector per Wintgen position in the uni-arm description. A complete set of inequivalent irreps of $\mathcal{G}$ is obtained from these irreps by varying the parameters within their ranges.

Data on the independent parameter ranges are essential to make sure that exactly one $\mathbf{k}$ vector per orbit is represented in the representation domain Φ or in the asymmetric unit. Such data are often much easier to calculate for the asymmetric unit of the unit cell than for the representation domain of the Brillouin zone, in particular if a uni-arm description has been chosen, *cf.* Section 1.5.5. Such data can not be found in the cited tables of irreps.

The uni-arm description unmasks those $\mathbf{k}$ vectors which lie on the boundary of the Brillouin zone but belong to a Wintgen position which also contains inner $\mathbf{k}$ vectors, see the example of the lines Λ and F in $(Fm\overline{3}m)^*$ and $(Fm\overline{3})^*$. Such $\mathbf{k}$ vectors can not give rise to little-group representations obtained from projective representations of the little co-group $\overline{\mathcal{G}}^{\mathbf{k}}$.

The consideration of the basic domain Ω in relation to the representation domain Φ is unnecessary. It may even be misleading because special $\mathbf{k}$-vector subspaces of Ω frequently belong to more general types of $\mathbf{k}$ vectors in Φ. 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.

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. Moreover, it is not difficult to relate one approach to the other, see Figs. and Tables 1.5.5.1 to 1.5.5.7. The conclusions show that the crystallographic approach for the description of irreps of space groups has several advantages as compared with the traditional 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 $\mathbf{k}$ 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 in order to find the optimal way to solve the problem.

The crystallographic approach may be realized in three different ways:

(1) In the *uni-arm description* one lists each $\mathbf{k}$-vector star exactly once by indicating the parameter field of the representing $\mathbf{k}$ vector. Advantages are the transparency of the presentation and the relatively small effort for the derivation of the list. A disadvantage may be that there are protruding flagpoles or wings. Points of flagpoles or wings 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.

(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 A1.5.1
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 $\mathcal{G}_0(\mathcal{G})$. For most space groups $\mathcal{G}$, the reciprocal-space group $(\mathcal{G})^*$ is isomorphic to $\mathcal{G}_0(\mathcal{G})$, *i.e.* $\mathcal{G}_0(\mathcal{G})$ and $(\mathcal{G})^*$ belong to the same arithmetic crystal class. In the following cases $(\mathcal{G})^*$ is isomorphic to a symmorphic space group $\mathcal{G}_0$ which is different from $\mathcal{G}_0(\mathcal{G})$. Thus 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, *e.g.* $(\mathcal{G})^*$ is isomorphic to $Imm2$ for the arithmetic crystal class $\mathcal{G} = mm2F$. 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 8.2.3):

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

References

Altmann, S. L. (1977). *Induced Representations in Crystals and Molecules.* London: Academic Press.

Aroyo, M. I., Kirov, A., Capillas, C., Perez-Mato, J. M. & Wondratschek, H. (2006). *Bilbao Crystallographic Server. II. Representations of crystallographic point groups and space groups. Acta Cryst.* A**62**, 115–128.

Aroyo, M. I., Perez-Mato, J. M., Capillas, C., Kroumova, E., Ivantchev, S., Madariaga, G., Kirov, A. & Wondratschek, H. (2006). *Bilbao Crystallographic Server: I. Databases and crystallographic computing programs. Z. Kristallogr.* **221**, 15–27.

Aroyo, M. I. & Wondratschek, H. (1995). *Crystallographic viewpoints in the classification of space-group representations. Z. Kristallogr.* **210**, 243–254.

Bilbao Crystallographic Server (1998). http://www.cryst.ehu.es/.

Bouckaert, L. P., Smoluchowski, R. & Wigner, E. P. (1936). *Theory of Brillouin zones and symmetry properties of wave functions in crystals. Phys. Rev.* **50**, 58–67.

Boyle, L. L. (1986). *The classification of space group representations.* In *Proceedings of the 14th International Colloquium on Group-Theoretical Methods in Physics*, pp. 405–408. Singapore: World Scientific.

Bradley, C. J. & Cracknell, A. P. (1972). *The Mathematical Theory of Symmetry in Solids: Representation Theory for Point Groups and Space Groups.* Oxford: Clarendon Press.

Cracknell, A. P., Davies, B. L., Miller, S. C. & Love, W. F. (1979). *Kronecker Product Tables*, Vol. 1, *General Introduction and Tables of Irreducible Representations of Space Groups.* New York: IFI/Plenum.

Davies, B. L. & Cracknell, A. P. (1976). *Some comments on and addenda to the tables of irreducible representations of the classical space groups published by S. C. Miller and W. F. Love. Acta Cryst.* A**32**, 901–903.

Davies, B. L. & Dirl, R. (1987). *Various classification schemes for irreducible space group representations.* In *Proceedings of the 15th International Colloquium on Group-Theoretical Methods in Physics*, edited by R. Gilmore, pp. 728–733. Singapore: World Scientific.

Delaunay, B. (1933*a*). *Neue Darstellung der geometrischen Kristallographie. Z. Kristallogr.* **84**, 109–149.

Delaunay, B. (1933*b*). *Berichtigung zur Arbeit "Neue Darstellung der geometrischen Kristallographie". Z. Kristallogr.* **85**, 332.

International Tables for Crystallography (2005). Vol. A, *Space-Group Symmetry*, edited by Th. Hahn, 5th ed. Heidelberg: Springer.

Jan, J.-P. (1972). *Space groups for Fermi surfaces. Can. J. Phys.* **50**, 925–927.

Jansen, L. & Boon, M. (1967). *Theory of Finite Groups. Applications in Physics: Symmetry Groups of Quantum Mechanical Systems.* Amsterdam: North-Holland.

Janssen, T. (2003). *International Tables for Crystallography*, Vol. D, *Physical Properties of Crystals*, edited by A. Authier, ch. 1.2, *Representations of crystallographic groups.* Dordrecht: Kluwer Academic Publishers.

Kovalev, O. V. (1986). *Irreducible and Induced Representations and Co-representations of Fedorov Groups.* Moscow: Nauka.

Lomont, J. S. (1959). *Applications of Finite Groups.* New York: Academic Press.

Miller, S. C. & Love, W. F. (1967). *Tables of Irreducible Representations of Space Groups and Co-representations of Magnetic Space Groups.* Boulder: Pruett Press.

Raghavacharyulu, I. V. V. (1961). *Representations of space groups. Can. J. Phys.* **39**, 830–840.

Rosen, J. (1981). *Resource letter SP-2: Symmetry and group theory in physics. Am. J. Phys.* **49**, 304–319.

Slater, L. S. (1962). *Quantum Theory of Molecules and Solids*, Vol. 2. Amsterdam: McGraw-Hill.

Smith, J. V. (1982). *Geometrical and Structural Crystallography*. New York: John Wiley & Sons.

Stokes, H. T. & Hatch, D. M. (1988). *Isotropy Subgroups of the 230 Crystallographic Space Groups.* Singapore: World Scientific.

Stokes, H. T., Hatch, D. M. & Nelson, H. M. (1993). *Landau, Lifshitz, and weak Lifshitz conditions in the Landau theory of phase transitions in solids. Phys. Rev. B*, **47**, 9080–9083.

Wintgen, G. (1941). *Zur Darstellungstheorie der Raumgruppen. Math. Ann.* **118**, 195–215.

Zak, J., Casher, A., Glück, M. & Gur, Y. (1969). *The Irreducible Representations of Space Groups.* New York: Benjamin.