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

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1.5.1. List of symbols

$\mathcal{G}$; $\mathcal{S}$	Group, especially space group; site-symmetry group
G	Element of group $\mathcal{G}$
$\mathcal{G}_0$	Symmorphic space group
$\mathcal{P}$ or $\bar{\mathcal{G}}$	Point group of space group $\mathcal{G}$
$\mathcal{T}$	Translation subgroup of space group $\mathcal{G}$
$\boldsymbol{R}, \boldsymbol{S}$; $\boldsymbol{W}$	Matrix; matrix part of a symmetry operation
$\boldsymbol{w}$	Column part of a symmetry operation
X	Point of point space
x, y, z; x_i	Coordinates of a point or coefficients of a vector
$\boldsymbol{x}$	Column of point coordinates or of vector coefficients
L	Vector lattice of the space group $\mathcal{G}$
$\mathbf{a}, \mathbf{b}, \mathbf{c}$ or $(\mathbf{a}_k)^T$	Basis vectors or row of basis vectors of the lattice **L** of $\mathcal{G}$
t	Vector of the lattice **L** of $\mathcal{G}$
$\mathbf{L}^*$	Reciprocal lattice of the space group $\mathcal{G}$
$\mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*$ or $(\mathbf{a}_k^*)$	Basis vectors or column of basis vectors of the reciprocal lattice $\mathbf{L}^*$
K	Vector of the reciprocal lattice $\mathbf{L}^*$
k	Vector of reciprocal space
$\mathcal{G}^*$	Reciprocal-space group
$\bar{\mathcal{G}}^{\mathbf{k}}$	Little co-group of **k**
$\mathcal{L}^{\mathbf{k}}$	Little group of **k**
$\Gamma(\mathcal{G})$	(Matrix) representation of $\mathcal{G}$

1.5.2. Introduction

This new 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 different numbers of types and 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 symmetry types 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) (1995) 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 50 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 $Pm\bar{3}m$. Similarly, Jan (1972) compared Wyckoff positions with points of the Brillouin zone when describing the symmetry $Pm\bar{3}$ 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 the 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 types of **k** vectors and symbols for them are introduced.

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

In this chapter 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. The consequences and advantages of this approach are demonstrated and discussed using examples in Section 1.5.5.

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 Bradley & Cracknell (1972) or the forthcoming Chapter 1.2 of *IT* D (*Physical properties of crystals*) by Janssen (2001).

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 irreducible representations are known. Naturally, the question of how to construct all nonequivalent irreducible representations 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 W of space groups $\mathcal{G}$ are nonlinear operations. The same holds for their description by matrix-column pairs $(\boldsymbol{W}, \boldsymbol{w})$,† 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.

† In physics often written as the Seitz symbol $(\boldsymbol{W}|\boldsymbol{w})$.

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.

To each space group $\mathcal{G}$ belongs an infinite set $\mathcal{T}$ of translations, the *translation lattice* of $\mathcal{G}$. The lattice $\mathcal{T}$ 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 elements W, *i.e.* the symmetry operations 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 left cosets relative to $\mathcal{T}$:

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

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 $\boldsymbol{o}$ 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 $\bar{\mathcal{G}}$ in books on representation theory) describing the symmetry of the external shape of the macroscopic crystal and being represented by the matrices $\boldsymbol{W}_1, \boldsymbol{W}_2, \ldots, \boldsymbol{W}_n$. 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 $\mathcal{G}_0$.

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 8.2.2; see also Section 8.3.4 and Table 8.2.

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. One assumes the Born–von Karman boundary conditions

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

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 $(\boldsymbol{I}, \boldsymbol{t})$,

$$(\boldsymbol{I}, \boldsymbol{Nt}) = (\boldsymbol{I}, \boldsymbol{o}) \qquad (1.5.3.3)$$

holds, where $\boldsymbol{Nt}$ 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 irreducible representations (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

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

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):

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

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

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

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

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 transposed. 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.

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

† In crystallography vectors are designated by small bold-faced letters. With $\mathbf{K}$ we make an exception in order to follow the tradition of physics. A crystallographic alternative would be $\mathbf{t}^*$.

‡ 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.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

1.5.4. Conventions in the classification of space-group irreps

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

1.5.4.1. *Fundamental regions*

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

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

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

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

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

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

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

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

1.5.4.2. *Minimal domains*

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

1.5.4.3. *Wintgen positions*

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

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

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

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

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

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

Comparison of the **k**-vector labels and parameters of CDML with the Wyckoff positions of *IT* A for $Fm\bar{3}m$, (O_h^5), isomorphic to the reciprocal-space group $\mathcal{G}^*$ of $m\bar{3}ml$. The parameter ranges in the last column are chosen such that each star of **k** is represented exactly once. The sign $\sim$ means symmetrically equivalent. The coordinates x, y, z of *IT* A are related to the **k**-vector coefficients of CDML by $x = 1/2(k_2 + k_3)$, $y = 1/2(k_1 + k_3)$, $z = 1/2(k_1 + k_2)$.

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

For non-holosymmetric space groups the representation domain Φ is a multiple of the basic domain Ω. CDML introduced new letters for stars of **k** vectors in those parts of Φ which do not belong to Ω. If one can make a new **k** vector uni-arm to some **k** vector of the basic domain Ω by an appropriate choice of Φ and Ω, one can extend the parameter range of this **k** vector of Ω to Φ instead of introducing new letters. It turns out that indeed most of these new letters are unnecessary. This restricts the introduction of new types of **k** vectors to the few cases where it is indispensible. Extension of the parameter range for **k** means that the corresponding representations can also be obtained by parameter variation. Such representations can be considered to belong to the same type. In this way a large number of superfluous **k**-vector names, which pretend a greater variety of types of irreps than really exists, can be avoided (Boyle, 1986). For examples see Section 1.5.5.1.

1.5.5. Examples and conclusions

1.5.5.1. *Examples*

In this section, four examples are considered in each of which the *crystallographic* classification scheme for the irreps is compared with the *traditional* one:†

(1) **k**-vector types of the arithmetic crystal class $m\bar{3}mI$ (space groups $Im\bar{3}m$ and $Ia\bar{3}d$), reciprocal-space group isomorphic to $Fm\bar{3}m$; $\Phi = \Omega$; see Table 1.5.5.1 and Fig. 1.5.5.1;

(2) **k**-vector types of the arithmetic crystal class $m\bar{3}I$ ($Im\bar{3}$ and $Ia\bar{3}$), reciprocal-space group isomorphic to $Fm\bar{3}$, $\Phi > \Omega$; see Table 1.5.5.2 and Fig. 1.5.5.2;

(3) **k**-vector types of the arithmetic crystal class $4/mmmI$ ($I4/mmm, I4/mcm, I4_1/amd$ and $I4_1/acd$), reciprocal-space group isomorphic to $I4/mmm$. Here $\Phi = \Omega$ changes for different ratios of the lattice constants a and c; see Table 1.5.5.3 and Fig. 1.5.5.3;

(4) **k**-vector types of the arithmetic crystal class *mm2F* (*Fmm2* and *Fdd2*), reciprocal-space group isomorphic to *Imm2*. Here $\Phi > \Omega$ changes for different ratios of the lattice constants a, b and c; see Table 1.5.5.4 and Fig. 1.5.5.4.

The asymmetric units of *IT* A are displayed in Figs. 1.5.5.1 to 1.5.5.4 by dashed lines. In Tables 1.5.5.1 to 1.5.5.4, the **k**-vector types of CDML are compared with the Wintgen (Wyckoff) positions of *IT* A. The parameter ranges are chosen such that each star of **k** is represented exactly once. Sets of symmetry points, lines or planes of CDML which belong to the same Wintgen position are separated by horizontal lines in Tables 1.5.5.1 to 1.5.5.3. The uni-arm description is listed in the last entry of each Wintgen position in Tables 1.5.5.1 and 1.5.5.2. In Table 1.5.5.4, so many **k**-vector types of CDML belong to each Wintgen position that the latter are used as headings under which the CDML types are listed.

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

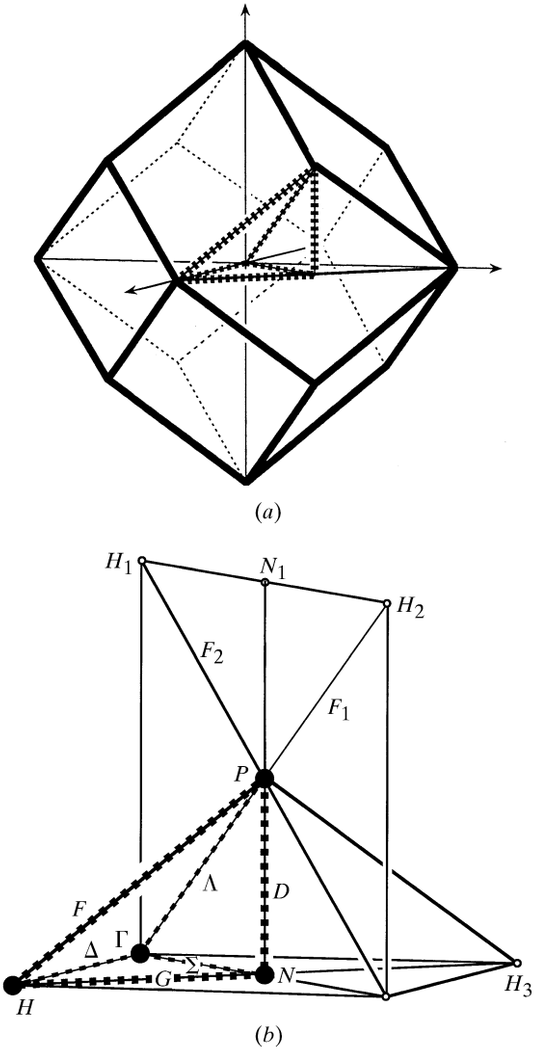

Fig. 1.5.5.1. Symmorphic space group $Fm\bar{3}m$ (isomorphic to the reciprocal-space group $\mathcal{G}^*$ of $m\bar{3}mI$). (*a*) The asymmetric unit (thick dashed edges) imbedded in the Brillouin zone, which is a cubic rhombdodecahedron. (*b*) The asymmetric unit ΓHNP, *IT* A, p. 678. The representation domain ΓNH_3P of CDML is obtained by reflecting ΓHNP through the plane of ΓNP. Coordinates of the *points*: $\Gamma = 0,0,0$; $N = \frac{1}{4},\frac{1}{4},0 \sim N_1 = \frac{1}{4},\frac{1}{4},\frac{1}{2}$; $H = \frac{1}{2},0,0 \sim H_1 = 0,0,\frac{1}{2} \sim H_2 = \frac{1}{2},\frac{1}{2},\frac{1}{2} \sim H_3 = 0,\frac{1}{2},0$; $P = \frac{1}{4},\frac{1}{4},\frac{1}{4}$; the sign $\sim$ means symmetrically equivalent. *Lines*: $\Lambda = \Gamma P = x,x,x$; $F = HP = \frac{1}{2}-x,x,x \sim F_1 = PH_2 = x,x,x \sim F_2 = PH_1 = x,x,\frac{1}{2}-x$; $\Delta = \Gamma H = x,0,0$; $\Sigma = \Gamma N = x,x,0$; $D = NP = \frac{1}{4},\frac{1}{4},z$; $G = NH = x,\frac{1}{2}-x,0$. *Planes*: $\mathrm{A} = \Gamma HN = x,y,0$; $B = HNP = x,\frac{1}{2}-x,z \sim PN_1H_1 = x,x,z$; $C = \Gamma NP = x,x,z$; $J = \Gamma HP = x,y,y \sim \Gamma PH_1 = x,x,z$. Large black circles: corners of the asymmetric unit (special points); small open circles: other special points; dashed lines: edges of the asymmetric unit (special lines). For the parameter ranges see Table 1.5.5.1.

1.5.5.2. *Results*

(1) The higher the symmetry of the point group $\bar{\mathcal{G}}$ of $\mathcal{G}$, the more one is restricted in the choice of the boundaries of the minimal domain. This is because a symmetry element (rotation or rotoinversion axis, plane of reflection, centre of inversion) cannot occur in the interior of the minimal domain but only on its boundary. However, even for holosymmetric space groups of highest symmetry, the description by Brillouin zone and representation domain is not as concise as possible, *cf.* CDML.

Examples:

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

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

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

(*b*) In Table 1.5.5.1 for $m\bar{3}mI$, see also Fig. 1.5.5.1, the $\mathbf{k}$-vector planes $B = HNP$, $C = \Gamma NP$ and $J = \Gamma HP$ of CDML belong to the same Wintgen position 96 *k* ..*m*. In the asymmetric unit of *IT* A (as in the representation domain of CDML) the plane *x*, *x*, *z* is kinked into parts belonging to different arms of the star of $\mathbf{k}$. Transforming, *e.g.*, *B* and *J* to the plane of *C* by $\mathbf{2}\ \frac{1}{4},y,\frac{1}{4}(B \rightarrow PN_1H_1)$ and $\mathbf{3}^-\ x,x,x\ (J \rightarrow \Gamma PH_1)$, one obtains a complete plane (ΓNN_1H_1 for *C*, *B* and *J*) as a uni-arm description of the Wintgen position 96 *k* ..*m*. This plane protrudes from the body of the asymmetric unit like a wing.

Remark. One should avoid the term *equivalent* for the relation between Λ and *F* or between *B*, *C* and *J* as it is used by Stokes *et al.* (1993). BC, p. 95 give the definition: 'Two $\mathbf{k}$ vectors $\mathbf{k}_1$ and $\mathbf{k}_2$ are equivalent if $\mathbf{k}_1 = \mathbf{k}_2 + \mathbf{K}$, where $\mathbf{K} \in \mathbf{L}^*$'. One can also express this by saying: 'Two $\mathbf{k}$ vectors are equivalent if they differ by a vector $\mathbf{K}$ of the (reciprocal) lattice.' We prefer to extend this equivalence by saying: 'Two $\mathbf{k}$ vectors $\mathbf{k}_1$ and $\mathbf{k}_2$ are equivalent if and only if they belong to the same orbit of $\mathbf{k}$', *i.e.* if there is a matrix part $\boldsymbol{W}$ and a vector $\mathbf{K} \in \mathbf{L}^*$ belonging to $\mathcal{G}^*$ such that $\mathbf{k}_2 = \boldsymbol{W}\mathbf{k}_1 + \mathbf{K}$, see equation (1.5.3.13). Alternatively, this can be expressed as: 'Two $\mathbf{k}$ vectors are equivalent if and only if they belong to the same or to translationally equivalent stars of $\mathbf{k}$.' The $\mathbf{k}$ vectors of Λ and *F* or of *B*, *C* and *J* are not even equivalent under this broader definition, see Davies & Dirl (1987). If the representatives of the $\mathbf{k}$-vector stars are chosen uni-arm, as in the examples, their non-equivalence is evident.

(2) In general two trends can be observed:

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

Examples:

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

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

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

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

the reciprocal-space group $(F4/mmm)^*$ (setting $I4/mmm$) are listed in Table 1.5.5.3. The main condition of the representation domain is that of the boundary plane $x, y, z = \{1 + (c/a)^2[1 - 2(x + y)]\}/4$, which for $c/a < 1$ forms the triangle Z_0Z_1P (Figs. 1.5.5.3*a*,*b*) but for $c/a > 1$ forms the pentagon S_1RPGS (Figs. 1.5.5.3*c*,*d*). The inner points of these boundary planes are points of the general position *GP* with the exception of the line $Q = x, \frac{1}{2} - x, \frac{1}{4}$, which is a twofold rotation axis. The boundary conditions for the representation domain depend on c/a; they are much more complicated than those for the asymmetric unit (for this the boundary condition is simply $x, y, \frac{1}{4}$).

(ii) In the reciprocal-space group $(Imm2)^*$, see Figs. 1.5.5.4(*a*) to (*c*), the lines Λ and Q belong to Wintgen position 2 *a* *mm*2; *G* and *H* belong to 2 *b* *mm*2; Δ and *R*, Σ and *U*, *A* and *C*, and *B* and *D* belong to the general position *GP*. The decisive boundary plane is $x/a^2 + y/b^2 + z/c^2 = d^2/4$, where $d^2 = 1/a^2 + 1/b^2 + 1/c^2$, or $xa^{*2} + yb^{*2} + zc^{*2} = d^{*2}/4$, where $d^{*2} = a^{*2} + b^{*2} + c^{*2}$. There is no relation of the lattice constants for which all the above-mentioned lines are realized on the surface of the representation domain simultaneously, either two or three of them do not appear and the length of the others depends on the boundary plane; see Table 1.5.5.4 and Figs. 1.5.5.4(*a*) to (*c*). Again, the boundary conditions for the asymmetric unit are independent of the lattice parameters, all lines mentioned above are present and their parameters run from 0 to $\frac{1}{2}$.

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

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

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

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

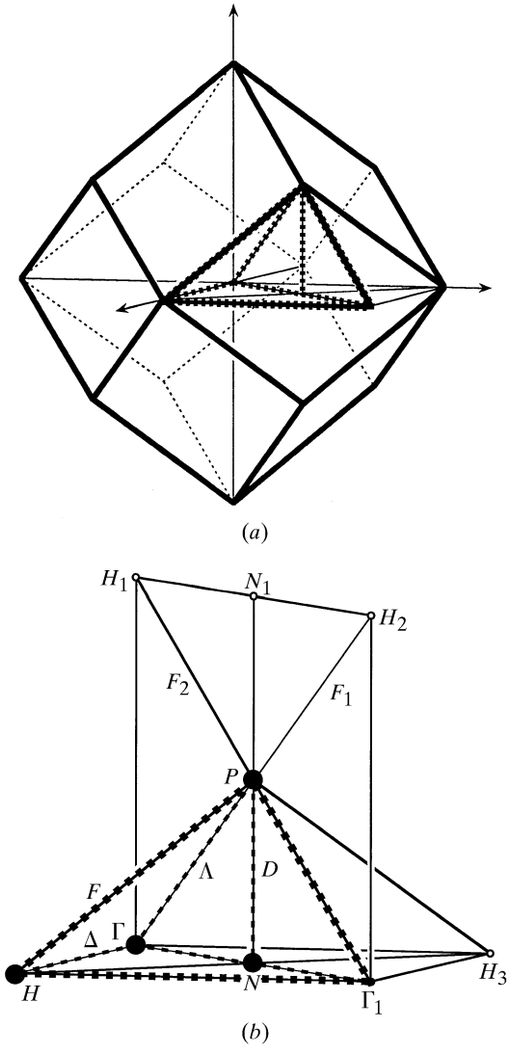

Fig. 1.5.5.2. Symmorphic space group $F\bar{3}m$ (isomorphic to the reciprocal-space group $\mathcal{G}^*$ of $m\bar{3}I$). (*a*) The asymmetric unit (thick dashed edges) half imbedded in and half protruding from the Brillouin zone, which is a cubic rhombdodecahedron (as in Fig. 1.5.5.1). (*b*) The asymmetric unit $\Gamma H\Gamma_1 P$, *IT* A, p. 610. The representation domain of CDML is ΓHH_3P. Both bodies have ΓHNP in common; $H\Gamma_1 NP$ is mapped onto ΓNH_3P by a twofold rotation around NP. The representation domain as the asymmetric unit would be the better choice because it is congruent to the asymmetric unit of *IT* A and is fully imbedded in the Brillouin zone. Coordinates of the *points*: $\Gamma = 0,0,0 \sim \Gamma_1 = \frac{1}{2},\frac{1}{2},0$; $P = \frac{1}{4},\frac{1}{4},\frac{1}{4}$; $H = \frac{1}{2},0,0 \sim H_1 = 0,0,\frac{1}{2} \sim H_2 = \frac{1}{2},\frac{1}{2},\frac{1}{2} \sim H_3 = 0,\frac{1}{2},0$; $N = \frac{1}{4},\frac{1}{4},0 \sim N_1 = \frac{1}{4},\frac{1}{4},\frac{1}{2}$; the sign $\sim$ means symmetrically equivalent. *Lines*: $\Lambda = \Gamma P = x,x,x \sim P\Gamma_1 = x,x,\frac{1}{2}-x$; $F = HP = \frac{1}{2}-x,x,x \sim F_1 = PH_2 = x,x,x \sim F_2 = PH_1 = x,x,\frac{1}{2}-x$; $\Delta = \Gamma H = x,0,0 \sim H\Gamma_1 = \frac{1}{2},y,0$; $D = PN = \frac{1}{4},\frac{1}{4},z$. ($G = NH = x,\ \frac{1}{2}-x,\ 0$ and $\Sigma = \Gamma N = x,x,0 \sim N\Gamma_1 = x,x,0$ are not special lines.) *Planes*: $A = \Gamma HN = x,y,0$; $AA = \Gamma_1 NH = x,y,0$; $B = HNP = x,\frac{1}{2}-x,z \sim PN_1H_1 = x,x,z$; $C = \Gamma NP = x,x,z$; $J = \Gamma HP = x,y,y \sim \Gamma PH_1 = x,x,z$. (The boundary planes B, C and J are parts of the general position *GP*.) Large black circles: special points of the asymmetric unit; small black circle: special point $\Gamma_1 \sim \Gamma$; small open circles: other special points; dashed lines: edges and special line D of the asymmetric unit. The edge $\Gamma\Gamma_1$ is not a special line but is part of the boundary plane $A \cup AA$. For the parameter ranges see Table 1.5.5.2.

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

1.5.5.3. *Parameter ranges*

For the uni-arm description of a Wintgen position it is easy to check whether the parameter ranges for the general or special constituents of the representation domain or asymmetric unit have been stated correctly. For this purpose one may define the *field* of **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 inside the unit cell. The order of the little co-group $\bar{\mathcal{G}}^{\mathbf{k}}$ ($\bar{\mathcal{G}}^{\mathbf{k}}$ represents those operations which leave the field of **k** *fixed pointwise*) is divided by the order of the stabilizer [which is the set of all symmetry operations (*modulo* integer translations) that leave the field *invariant as a whole*]. The result gives the independent fraction of the above-determined volume of the unit cell or the area of the plane or length of the line.

If the description is not uni-arm, the uni-arm parameter range will be split into the parameter ranges of the different arms. The parameter ranges of the different arms are not necessarily equal; see the second of the following examples.

Examples:

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

(2) Plane $B \cup C \cup J$: In $(Fm\bar{3}m)^*$, the stabilizer of x, x, z is generated by $m.mm$ and the centring translation $t(\frac{1}{2},\frac{1}{2},0)$ modulo integer translations (mod $\mathbf{T}_{\rm int}$). They generate a group of order 16; $\bar{\mathcal{G}}^{\mathbf{k}}$ is $..m$ of order 2. The fraction of the plane is $\frac{2}{16} = \frac{1}{8}$ of the area $2^{1/2}a^{*2}$, as expressed by the parameter ranges $0 < x < \frac{1}{4}$, $0 < z < \frac{1}{2}$. There are six arms of the star of x,x,z: x,x,z; $\bar{x},x,z$; x,y,x; $x,y,\bar{x}$; x,y,y; $x,\bar{y},y$. Three of them are represented in the boundary of the representation domain: $B = HNP$, $C = \Gamma NP$ and $J = \Gamma HP$; see Fig. 1.5.5.1. The areas of their parameter ranges are $\frac{1}{32}$, $\frac{1}{32}$ and $\frac{1}{16}$, respectively; the sum is $\frac{1}{8}$.

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

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

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

Data for the independent parameter ranges are essential to make sure that exactly one **k** vector per orbit is represented in the representation domain Φ or in the asymmetric unit. Such data are

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

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

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

k-vector labels, CDML		Wyckoff position, *IT* A	Parameters (see Fig. 1.5.5.3), *IT* A	
$a > c$	$a < c$		$a > c$	$a < c$†
Γ 0, 0, 0	Γ 0, 0, 0	2 *a* $4/mmm$	0, 0, 0	
M $-\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	*M* $\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}$	2 *b* $4/mmm$	$\frac{1}{2}, \frac{1}{2}, 0$	$0, 0, \frac{1}{2}$
X $0, 0, \frac{1}{2}$	*X* $0, 0, \frac{1}{2}$	4 *c* *mmm.*	$0, \frac{1}{2}, 0$	
P $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	*P* $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	4 *d* $\bar{4}m2$	$0, \frac{1}{2}, \frac{1}{4}$	
N $0, \frac{1}{2}, 0$	*N* $0, \frac{1}{2}, 0$	8 *f* ..$2/m$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	
Λ $\alpha, \alpha, -\alpha$ *V* $-\frac{1}{2}+\alpha, \frac{1}{2}+\alpha, \frac{1}{2}-\alpha$	Λ $\alpha, \alpha, -\alpha$ —	4 *e* 4*mm* 4 *e* 4*mm*	0, 0, *z*: $0 < z \le z_0$‡ $\frac{1}{2}, \frac{1}{2}, z$: $0 < z < z_1 = \frac{1}{2} - z_0$	$0 < z < \frac{1}{2}$ —
W $\alpha, \alpha, \frac{1}{2}-\alpha$	*W* $\alpha, \alpha, \frac{1}{2}-\alpha$	8 *g* 2*mm.*	$0, \frac{1}{2}, z$: $0 < z < \frac{1}{4}$	
Σ $-\alpha, \alpha, \alpha$ —	Σ $-\alpha, \alpha, \alpha$ *F* $\frac{1}{2}-\alpha, \frac{1}{2}+\alpha, -\frac{1}{2}+\alpha$	8 *h* *m*.2*m* 8 *h* *m*.2*m*	$x, x, 0$: $0 < x < \frac{1}{2}$ —	$0 < x \le s_1$ $x, x, \frac{1}{2}$: $0 < x < s = \frac{1}{2} - s_1$
Δ 0, 0, α	Δ 0, 0, α	8 *i* *m*2*m.*	0, *y*, 0: $0 < y < \frac{1}{2}$	
Y $-\alpha, \alpha, \frac{1}{2}$ —	*Y* $-\alpha, \alpha, \frac{1}{2}$ *U* $\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}+\alpha$	8 *j* *m*2*m.* 8 *j* *m*2*m.*	$x, \frac{1}{2}, 0$: $0 < x < \frac{1}{2}$ —	$0 < x \le r$ $0, y, \frac{1}{2}$: $0 < y < g = \frac{1}{2} - r$
Q $\frac{1}{4}-\alpha, \frac{1}{4}+\alpha, \frac{1}{4}-\alpha$	*Q* $\frac{1}{4}-\alpha, \frac{1}{4}+\alpha, \frac{1}{4}-\alpha$	16 *k* ..2	$x, \frac{1}{2}-x, \frac{1}{4}$: $0 < x < \frac{1}{4}$	
C $-\alpha, \alpha, \beta$ —	*C* $-\alpha, \alpha, \beta$ *D* $\frac{1}{2}-\alpha, \frac{1}{2}+\alpha, -\frac{1}{2}+\beta$	16 *l* *m*.. 16 *l* *m*..	*x*, *y*, 0: $0 < x < y < \frac{1}{2}$§ —	— *x*, *y*, $\frac{1}{2}$
B $\alpha, \beta, -\alpha$	*B* $\alpha, \beta, -\alpha$	16 *m* ..*m*	*x*, *x*, *z*: $0 < x < \frac{1}{2}$, $0 < z < \frac{1}{4} \cup 0 < x < \frac{1}{4}$, $z = \frac{1}{4}$	
A α, α, β *E* $\alpha-\beta, \alpha+\beta, \frac{1}{2}-\alpha$	*A* α, α, β *E* $\alpha-\beta, \alpha+\beta, \frac{1}{2}-\alpha$	16 *n* .*m.* 16 *n* .*m.*	0, *y*, *z*: $0 < y < \frac{1}{2}$, $0 < z < \frac{1}{2}$¶ *x*, $\frac{1}{2}$, *z*: transferred to $A = 0, y, z$	
GP α, β, γ	*GP* α, β, γ	32 *o* 1	*x*, *y*, *z*: $0 < x < y < \frac{1}{2}$, $0 < z < \frac{1}{4} \cup 0 < x < y < \frac{1}{2} - x$, $z = \frac{1}{4}$	

† If the parameter range is different from that for $a > c$.
‡ z_0 is a coordinate of point Z_0 *etc.*, see Figs. 1.5.5.3(*b*), (*d*).
§ For $a < c$, the parameter range includes the equivalent of $D = MSG$.
¶ The parameter range includes *A* and the equivalent of *E*.

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

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

(5) Line *x*, *x*, *x*: In $(Fm\bar{3}m)$* and $(Fm\bar{3})$* the points 0, 0, 0; $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ (and $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$) are special points; the parameter ranges are open: $0 < x < \frac{1}{4}$, $\frac{1}{4} < x < \frac{1}{2}$.

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

(7) Plane *x*, *y*, 0: In both $(Fm\bar{3}m)^*$ and $(Fm\bar{3})^*$, $0 < x$ and $0 < y$ holds. The **k** vectors of line *x*, *x*, 0 have little co-groups of higher order and belong to another Wintgen position in the representation domain (or asymmetric unit) of $(Fm\bar{3}m)^*$. Therefore, *x*, *y*, 0 is open at its boundary *x*, *x*, 0 in the range $0 < x < \frac{1}{4}$. In the asymmetric unit of $(Fm\bar{3})^*$ the line *x*, *x*, 0: $0 < x < \frac{1}{4}$ belongs to the plane, in this range the boundary of plane *A* is closed. The other range *x*, *x*, 0: $\frac{1}{4} < x < \frac{1}{2}$ is equivalent to the range $0 < x < \frac{1}{4}$ and thus does not belong to the asymmetric unit; here the boundary of *AA* is open.

1.5.5.4. *Conclusions*

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

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

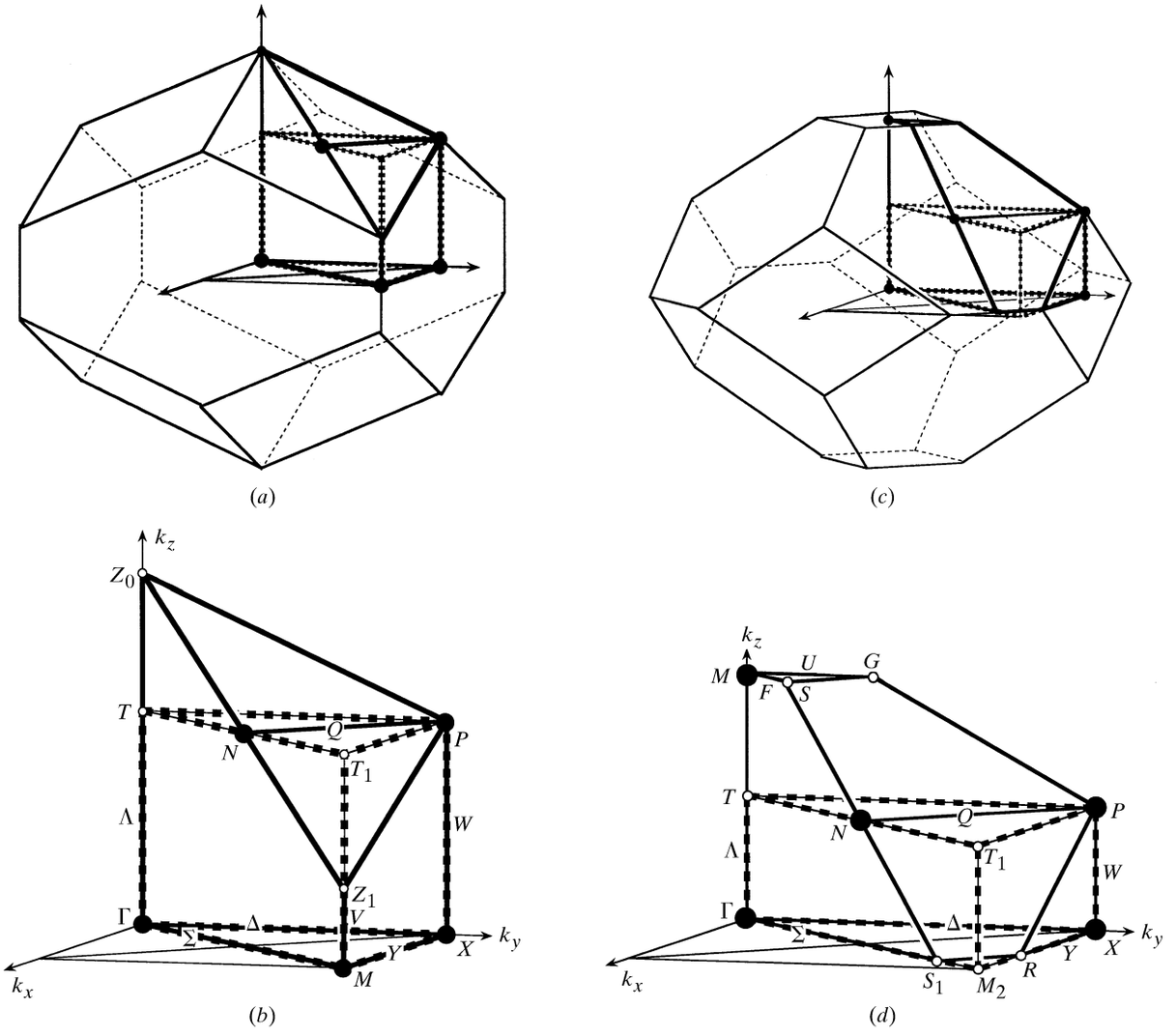

Fig. 1.5.5.3. (*a*), (*b*). Symmorphic space group $I4/mmm$ (isomorphic to the reciprocal-space group $\mathcal{G}^*$ of $4/mmmI$). Diagrams for $a > c$, *i.e.* $c^* > a^*$. In the figures $a = 1.25c$, *i.e.* $c^* = 1.25a^*$. (*a*) Representation domain (thick lines) and asymmetric unit (thick dashed lines, partly protruding) imbedded in the Brillouin zone, which is a tetragonal elongated rhombdodecahedron. (*b*) Representation domain ΓMXZ_1PZ_0 and asymmetric unit $\Gamma MXTT_1P$ of $I4/mmm$, *IT* A, p. 468. The part $\Gamma MXTNZ_1P$ is common to both bodies; the part $TNPZ_0$ is equivalent to the part NZ_1PT_1 by a twofold rotation around the axis $Q = NP$. Coordinates of the *points*: $\Gamma = 0,0,0$; $X = 0,\frac{1}{2},0$; $M = \frac{1}{2},\frac{1}{2},0$; $P = 0,\frac{1}{2},\frac{1}{4}$; $N = \frac{1}{4},\frac{1}{4},\frac{1}{4}$; $T = 0,0,\frac{1}{4} \sim T_1 = \frac{1}{2},\frac{1}{2},\frac{1}{4}$; $Z_0 = 0,0,z_0 \sim Z_1 = \frac{1}{2},\frac{1}{2},z_1$ with $z_0 = [1 + (c/a)^2]/4$; $z_1 = \frac{1}{2} - z_0$; the sign $\sim$ means symmetrically equivalent. *Lines*: $\Lambda = \Gamma Z_0 = 0,0,z$; $V = Z_1M = \frac{1}{2},\frac{1}{2},z$; $W = XP = 0,\frac{1}{2},z$; $\Sigma = \Gamma M = x,x,0$; $\Delta = \Gamma X = 0,y,0$; $Y = XM = x,\frac{1}{2},0$; $Q = PN = x,\frac{1}{2} - x,\frac{1}{4}$. The lines Z_0Z_1, Z_1P and PZ_0 have no special symmetry but belong to special planes. *Planes*: $C = \Gamma MX = x,y,0$; $B = \Gamma Z_0Z_1M = x,x,z$; $A = \Gamma XPZ_0 = 0,y,z$; $E = MXPZ_1 = x,\frac{1}{2},z$. The plane Z_0Z_1P belongs to the general position *GP*. Large black circles: special points belonging to the representation domain; small open circles: $T \sim T_1$ and $Z_0 \sim Z_1$ belonging to special lines; thick lines: edges of the representation domain and special line $Q = NP$; dashed lines: edges of the asymmetric unit. For the parameter ranges see Table 1.5.5.3.

(*c*), (*d*). Symmorphic space group $I4/mmm$ (isomorphic to the reciprocal-space group $\mathcal{G}^*$ of $4/mmmI$). Diagrams for $c > a$, *i.e.* $a^* > c^*$. In the figures $c = 1.25a$, *i.e.* $a^* = 1.25c^*$. (*c*) Representation domain (thick lines) and asymmetric unit (dashed lines, partly protruding) imbedded in the Brillouin zone, which is a tetragonal cuboctahedron. (*d*) Representation domain $\Gamma S_1RXPMSG$ and asymmetric unit ΓM_2XTT_1P of $I4/mmm$, *IT* A, p. 468. The part ΓS_1RXTNP is common to both bodies; the part $TNPMSG$ is equivalent to the part $T_1NPM_2S_1R$ by a twofold rotation around the axis $Q = NP$. Coordinates of the *points*: $\Gamma = 0,0,0$; $X = 0,\frac{1}{2},0$; $N = \frac{1}{4},\frac{1}{4},\frac{1}{4}$; $M = 0,0,\frac{1}{2} \sim M_2 = \frac{1}{2},\frac{1}{2},0$; $T = 0,0,\frac{1}{4} \sim T_1 = \frac{1}{2},\frac{1}{2},\frac{1}{4}$; $P = 0,\frac{1}{2},\frac{1}{4}$; $S = s,s,\frac{1}{2} \sim S_1 = s_1,s_1,0$ with $s = [1 - (a/c)^2]/4$; $s_1 = \frac{1}{2} - s$; $R = r,\frac{1}{2},0 \sim G = 0,g,\frac{1}{2}$ with $r = (a/c)^2/2$; $g = \frac{1}{2} - r$; the sign $\sim$ means symmetrically equivalent. *Lines*: $\Lambda = \Gamma M = 0,0,z$; $W = XP = 0,\frac{1}{2},z$; $\Sigma = \Gamma S_1 = x,x,0$; $F = MS = x,x,\frac{1}{2}$; $\Delta = \Gamma X = 0,y,0$; $Y = XR = x,\frac{1}{2},0$; $U = MG = 0,y,\frac{1}{2}$; $Q = PN = x,\frac{1}{2} - x,\frac{1}{4}$. The lines $GS \sim S_1R$, $SN \sim NS_1$ and $GP \sim PR$ have no special symmetry but belong to special planes. *Planes*: $C = \Gamma S_1RX = x,y,0$; $D = MSG = x,y,\frac{1}{2}$; $B = \Gamma S_1SM = x,x,z$; $A = \Gamma XPGM = 0,y,z$; $E = RXP = x,\frac{1}{2},z$. The plane S_1RPGS belongs to the general position *GP*. Large black circles: special points belonging to the representation domain; small open circles: $M_2 \sim M$; the points $T \sim T_1$, $S \sim S_1$ and $G \sim R$ belong to special lines; thick lines: edges of the representation domain and special line $Q = NP$; dashed lines: edges of the asymmetric unit. For the parameter ranges see Table 1.5.5.3.

Table 1.5.5.4. *The* **k***-vector types for the space groups Fmm*2 *and Fdd*2

Comparison of the **k**-vector labels and parameters of CDML with the Wyckoff positions of *IT* A for *Imm*2 (C_{2h}^{20}), isomorphic to the reciprocal-space group $\mathcal{G}^*$ of *mm2F*. For the asymmetric unit see Fig. 1.5.5.4. Four ratios of the lattice constants are distinguished in CDML, Fig. 3.6 for the representation domains: (*a*) $a^{*2} < b^{*2} + c^{*2}$, $b^{*2} < c^{*2} + a^{*2}$ and $c^{*2} < a^{*2} + b^{*2}$ (see Fig. 1.5.5.4*a*); (*b*) $c^{*2} > a^{*2} + b^{*2}$ (see Fig. 1.5.5.4*b*); (*c*) $b^{*2} > c^{*2} + a^{*2}$ [not displayed because essentially the same as (*d*)]; (*d*) $a^{*2} > b^{*2} + c^{*2}$ (see Fig. 1.5.5.4*c*). The vertices of the Brillouin zones of Fig. 3.6(*a*)–(*d*) with a variable coordinate are not designated in CDML. In Figs. 1.5.5.4 (*a*), (*b*) and (*c*) they are denoted as follows: the end point of the line Λ is Λ_0, of line Δ is Δ_0, of line Σ is Σ_0, of line A is A_0 *etc.* The variable coordinate of the end point is λ_0, δ_0, σ_0, a_0 *etc*., respectively. The line A_0B_0 is called *ab etc.* The plane (111) is called φ. It has the equation in the $\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$ basis φ: $a^{*2}x + b^{*2}y + c^{*2}z = d^{*2}/4$ with $d^{*2} = a^{*2} + b^{*2} + c^{*2}$. From this equation one calculates the variable coordinates of the vertices of the Brillouin zone: $\Lambda_0\ \ 0, 0, \lambda_0$ with $\lambda_0 = d^{*2}/4c^{*2}$; $Q_0\ \ \frac{1}{2}, \frac{1}{2}, q_0$ with $q_0 = \frac{1}{2} - \lambda_0$; $\Delta_0\ \ 0, \delta_0, 0$ with $\delta_0 = d^{*2}/4b^{*2}$; $R_0\ \ \frac{1}{2}, r_0, \frac{1}{2}$ with $r_0 = \frac{1}{2} - \delta_0$; $\Sigma_0\ \ \sigma_0, 0, 0$ with $\sigma_0 = d^{*2}/4a^{*2}$; $U_0\ \ u_0, \frac{1}{2}, \frac{1}{2}$ with $u_0 = \frac{1}{2} - \sigma_0$; $A_0\ \ a_0, 0, \frac{1}{2}$ with $a_0 = \frac{1}{4} + (b^{*2} - c^{*2})/4a^{*2}$; $C_0\ \ c_0, \frac{1}{2}, 0$ with $c_0 = \frac{1}{2} - a_0$; $B_0\ \ 0, b_0, \frac{1}{2}$ with $b_0 = \frac{1}{4} + (a^{*2} - c^{*2})/4b^{*2}$; $D_0\ \ \frac{1}{2}, d_0, 0$ with $d_0 = \frac{1}{2} - b_0$; $G_0\ \ \frac{1}{2}, 0, g_0$ with $g_0 = \frac{1}{4} + (b^{*2} - a^{*2})/4c^{*2}$; $H_0\ \ 0, \frac{1}{2}, h_0$ with $h_0 = \frac{1}{2} - g_0$. The coordinates x, y, z of *IT* A are related to the **k**-vector coefficients of CDML by $x = 1/2(-k_1 + k_2 + k_3)$, $y = 1/2(k_1 - k_2 + k_3)$, $z = 1/2(k_1 + k_2 - k_3)$. If necessary, a lattice vector has been added or a twofold screw rotation around the axis $\frac{1}{4}, \frac{1}{4}, z$ has been performed in order to shift the range of coordinates to $0 \le x, y, z \le \frac{1}{2}$. For example, $-\alpha, -\alpha, 0 \sim 0, 0, -z'$ with $0 < z' < \lambda_0$ is replaced by $\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z' = \frac{1}{2}, \frac{1}{2}, z$ with $\frac{1}{2} - \lambda_0 < z < \frac{1}{2}$. (The sign $\sim$ means symmetrically equivalent.)

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

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

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

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

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

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

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

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

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

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

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

In principle, both approaches are equivalent: the *traditional* one by Brillouin zone, basic domain and representation domain, and the *crystallographic* one by unit cell and asymmetric unit of *IT* A. Moreover, it is not difficult to relate one approach to the other, see the figures and Tables 1.5.5.1 to 1.5.5.4. The conclusions show that the *crystallographic* approach for the description of irreps of space groups has several advantages as compared to the *traditional*

Table 1.5.5.4. *The* **k***-vector types for the space groups Fmm*2 *and Fdd*2 (*cont.*)

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

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

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

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

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

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

k-vector label, CDML	Type of Brillouin zone as in:					
	Fig. 1.5.5.4(*a*)		Fig. 1.5.5.4(*b*)		Fig. 1.5.5.4(*c*)	
	CDML	*IT* A	CDML	*IT* A	CDML	*IT* A
GP	α, β, γ	x, y, z	α, β, γ	x, y, z	α, β, γ	x, y, z

approach. Owing to these advantages, CDML have already accepted the crystallographic approach for triclinic and monoclinic space groups. However, the advantages are not restricted to such low symmetries. In particular, the simple boundary conditions and shapes of the asymmetric units result in simple equations for the boundaries and shapes of volume elements, and facilitate numerical calculations, integrations *etc.* If there are special reasons to prefer **k** vectors inside or on the boundary of the Brillouin zone to those outside, then the advantages and disadvantages of both approaches have to be compared again in order to find the optimal method for the solution of the problem.

The crystallographic approach may be realized in three different ways:

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

relatively small effort required to derive the list. A disadvantage may be that there are protruding flagpoles or wings. Points of these lines or planes are no longer neighbours of inner points (an inner point has a full three-dimensional sphere of neighbours which belong to the asymmetric unit).

(2) In the *compact description* one lists each **k** vector exactly once such that each point of the asymmetric unit is either an inner point itself or has inner points as neighbours. Such a description may not be uni-arm for some Wintgen positions, and the determination of the parameter ranges may become less straightforward. Under this approach, all points fulfil the conditions for the asymmetric units of *IT* A, which are always closed. The boundary conditions of *IT* A have to be modified: in reality the boundary is not closed everywhere; there are frequently open parts (see Section 1.5.5.3).

(3) In the *non-unique description* one gives up the condition that each **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 **k** vectors which occur in more than one entry. Such tables are most informative and not too complicated for practical applications.

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Appendix 1.5.1.

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

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

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

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

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

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

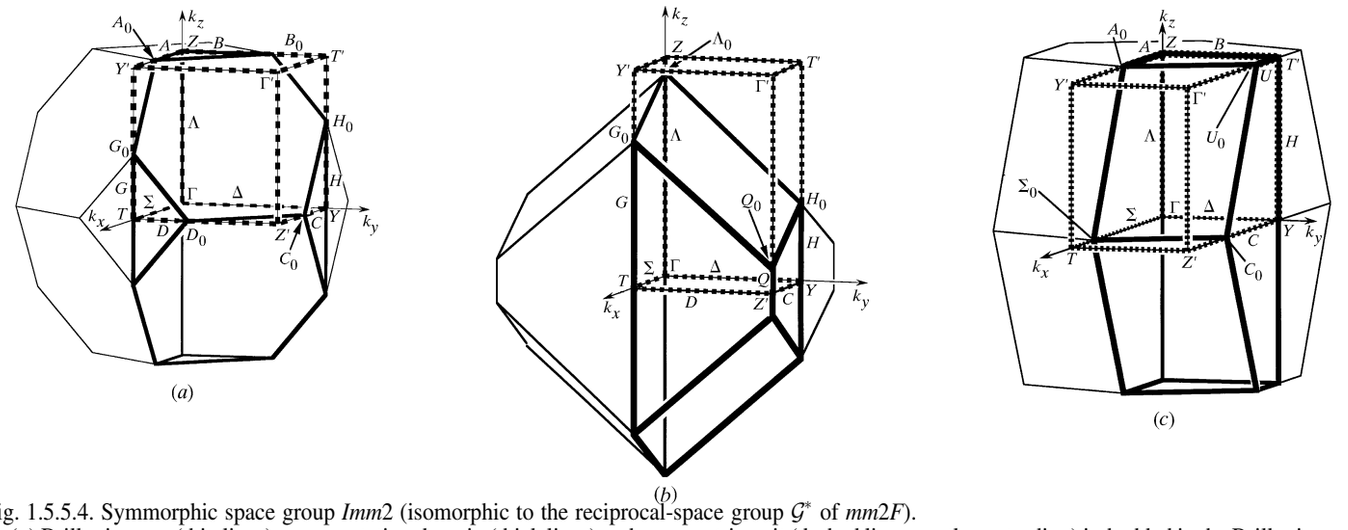

Fig. 1.5.5.4. Symmorphic space group *Imm*2 (isomorphic to the reciprocal-space group $\mathcal{G}^*$ of *mm*2*F*).

(*a*) Brillouin zone (thin lines), representation domain (thick lines) and asymmetric unit (dashed lines, partly protruding) imbedded in the Brillouin zone, which is an orthorhombic cuboctahedron. The diagram is drawn for $a^{*2} = 9$, $b^{*2} = 8$, $c^{*2} = 7$, *i.e.* $a^{*2} + b^{*2} > c^{*2}$. The endpoint of line *A* is A_0 *etc.*, the free coordinate of A_0 is a_0 *etc.* Asymmetric unit $\Gamma TZ'YZY'\Gamma'T'$ of *Imm*2, *IT* A, p. 246. The part $\Gamma TD_0C_0YG_0H_0ZA_0B_0$ is common to both bodies; the part $A_0Y'\Gamma'T'B_0G_0H_0D_0Z'C_0$ is equivalent to the part of the representation domain with negative z values through a twofold screw rotation 2_1 around the axis $\frac{1}{4}, \frac{1}{4}, z$. Coordinates of the *points*: $\Gamma = 0,0,0 \sim \Gamma' = \frac{1}{2},\frac{1}{2},\frac{1}{2}$; $Y = 0,\frac{1}{2},0 \sim Y' = \frac{1}{2},0,\frac{1}{2}$; $Z = 0,0,\frac{1}{2} \sim Z' = \frac{1}{2},\frac{1}{2},0$; $T = \frac{1}{2},0,0 \sim T' = 0,\frac{1}{2},\frac{1}{2}$; $C_0 = c_0,\frac{1}{2},0 \sim A_0 = a_0,0,\frac{1}{2}$; $D_0 = \frac{1}{2},d_0,0 \sim B_0 = 0,b_0,\frac{1}{2}$; $G_0 = \frac{1}{2},0,g_0 \sim H_0 = 0,\frac{1}{2},h_0$. The coordinates of the points are $c_0 = 1/4[1 - (b^{*2} - c^{*2})/a^{*2}]$; $a_0 = 1/2 - c_0$; $d_0 = 1/4[1 - (a^{*2} - c^{*2})/b^{*2}]$; $b_0 = 1/2 - d_0$; $g_0 = 1/4[1 - (a^{*2} - b^{*2})/c^{*2}]$; $h_0 = 1/2 - g_0$. The sign $\sim$ means symmetrically equivalent. There are no special points. The points Γ, *T*, *Y*, *Z*, G_0 and H_0 belong to special lines; A_0, B_0, C_0 and D_0 belong to special planes. The points with negative z coordinates are equivalent to those already listed. *Lines*: $\Lambda = \Gamma Z = 0,0,z$; $G = TG_0 = \frac{1}{2},0,z$; $H = YH_0 = 0,\frac{1}{2},z$. The lines $\Sigma = \Gamma T = x,0,0$; $C = YC_0 = x,\frac{1}{2},0$; $A = ZA_0 = x,0,\frac{1}{2}$; $\Delta = \Gamma Y = 0,y,0$; $B = ZB_0 = 0,y,\frac{1}{2}$; $D = TD_0 = \frac{1}{2},y,0$; A_0G_0, G_0D_0, C_0H_0 and H_0B_0 have no special symmetry but belong to special planes, the lines D_0C_0 and B_0A_0 belong to the general position *GP*. The lines $\Gamma\bar{Z}$, $T\bar{G}_0$, $Y\bar{H}_0$, $D_0\bar{G}_0$, $C_0\bar{H}_0$, $\bar{G}_0\bar{A}_0$, $\bar{H}_0\bar{B}_0$, $\bar{Z}\bar{A}_0$, $\bar{Z}\bar{B}_0$ and $\bar{A}_0\bar{B}_0$ of the representation domain to the points $\bar{Z}$, $\bar{G}_0$, $\bar{H}_0$, $\bar{A}_0$ and $\bar{B}_0$ with negative z coordinates are equivalent to lines of the asymmetric unit not belonging to the representation domain. *Planes*: $E = \Gamma YH_0B_0Z = 0,y,z$; $F = TD_0G_0 = \frac{1}{2},y,z$; $J = \Gamma ZA_0G_0T = x,0,z$; $K = YH_0C_0 = x,\frac{1}{2},z$. The planes x, y, 0; x, y, $\frac{1}{2}$; and $D_0C_0H_0B_0A_0G_0$ belong to the general position *GP*, as do the negative counterparts of the latter two. The planes $\Gamma\bar{Z}\bar{A}_0\bar{G}_0T$, $\Gamma\bar{Z}\bar{B}_0\bar{H}_0Y$, $Y\bar{H}_0C_0$ and $TD_0\bar{G}_0$ of the representation domain to the points $\bar{Z}$, $\bar{A}_0$, $\bar{B}_0$, $\bar{G}_0$ and $\bar{H}_0$ with negative z coordinates are equivalent to planes of the asymmetric unit not belonging to the representation domain. For the parameter ranges see Table 1.5.5.4.

(*b*) Brillouin zone (thin lines), representation domain (thick lines) and asymmetric unit (dashed lines, partly protruding) imbedded in the Brillouin zone, which is an orthorhombic elongated rhombdodecahedron. The diagram is drawn for $a^{*2} = 4$, $b^{*2} = 9$, $c^{*2} = 16$, *i.e.* $a^{*2} + b^{*2} < c^{*2}$. The endpoint of line *G* is G_0 *etc.*, the free coordinate of G_0 is g_0 *etc.* Asymmetric unit $\Gamma TZ'YZY'\Gamma'T'$ of *Imm*2, *IT* A, p. 246. The part $\Gamma TZ'YQ_0H_0\Lambda_0G_0$ is common to both bodies; the part $ZY'\Gamma'T'\Lambda_0G_0Q_0H_0$ is equivalent to the part of the representation domain with negative z values through a twofold screw rotation 2_1 around the axis $\frac{1}{4}, \frac{1}{4}, z$. Coordinates of the *points*: $\Gamma = 0,0,0 \sim \Gamma' = \frac{1}{2},\frac{1}{2},\frac{1}{2}$; $Y = 0,\frac{1}{2},0 \sim Y' = \frac{1}{2},0,\frac{1}{2}$; $Z = 0,0,\frac{1}{2} \sim Z' = \frac{1}{2},\frac{1}{2},0$; $T = \frac{1}{2},0,0 \sim T' = 0,\frac{1}{2},\frac{1}{2}$; $\Lambda_0 = 0,0,\lambda_0 \sim Q_0 = \frac{1}{2},\frac{1}{2},q_0$; $G_0 = \frac{1}{2},0,g_0 \sim H_0 = 0,\frac{1}{2},h_0$. The coordinates of the points are $\lambda_0 = 1/4[1 + (a^{*2} + b^{*2})/c^{*2}]$; $q_0 = 1/2 - \lambda_0$; $g_0 = 1/4[1 + (b^{*2} - a^{*2})/c^{*2}]$; $h_0 = 1/2 - g_0$. The sign $\sim$ means symmetrically equivalent. There are no special points. The points Γ, *T*, *Y*, *Z'*, Λ_0, Q_0, G_0 and H_0 belong to special lines. The points with negative z coordinates are equivalent to those already listed. *Lines*: $\Lambda = \Gamma\Lambda_0 = 0,0,z$; $Q = Z'Q_0 = \frac{1}{2},\frac{1}{2},z$; $G = TG_0 = \frac{1}{2},0,z$; $H = YH_0 = 0,\frac{1}{2},z$. The lines $\Sigma = \Gamma T = x,0,0$; $C = YZ' = x,\frac{1}{2},0$; $\Delta = \Gamma Y = 0,y,0$; $D = TZ' = \frac{1}{2},y,0$; Q_0G_0, $G_0\Lambda_0$, Λ_0H_0 and H_0Q_0 have no special symmetry but belong to special planes. The lines $\Gamma\bar{\Lambda}_0$, $Z'\bar{Q}_0$, $T\bar{G}_0$ and $Y\bar{H}_0$ of the representation domain to the points $\bar{\Lambda}$, $\bar{Q}_0$, $\bar{G}_0$ and $\bar{H}_0$ with negative z coordinates are equivalent to lines of the asymmetric unit not belonging to the representation domain. *Planes*: $E = \Gamma YH_0\Lambda_0 = 0,y,z$; $F = TZ'Q_0G_0 = \frac{1}{2},y,z$; $J = \Gamma\Lambda_0G_0T = x,0,z$; $K = YH_0Q_0Z' = x,\frac{1}{2},z$. The planes x, y, 0 and $\Lambda_0G_0Q_0H_0$ belong to the general position *GP*, as does the negative counterpart of $\Lambda_0G_0Q_0H_0$. The planes $\Gamma\bar{\Lambda}_0\bar{G}_0T$, $\Gamma\bar{\Lambda}_0\bar{H}_0Y$, $Y\bar{H}_0\bar{Q}_0Z'$ and $T\bar{G}_0\bar{Q}_0Z'$ of the representation domain to the points $\bar{\Lambda}$, $\bar{Q}_0$, $\bar{G}_0$ and $\bar{H}_0$ with negative z coordinates are equivalent to planes of the asymmetric unit not belonging to the representation domain. For the parameter ranges see Table 1.5.5.4.

(*c*) Brillouin zone (thin lines), representation domain (thick lines) and asymmetric unit (dashed lines, partly protruding) imbedded in the Brillouin zone, which is an orthorhombic elongated rhombdodecahedron. The diagram is drawn for $a^{*2} = 49$, $b^{*2} = 9$, $c^{*2} = 16$, *i.e.* $a^{*2} > b^{*2} + c^{*2}$. The endpoint of line *A* is A_0 *etc.*, the free coordinate of A_0 is a_0 *etc.* Asymmetric unit $\Gamma TZ'YZY'\Gamma'T'$ of *Imm*2, *IT* A, p. 246. The part $\Gamma\Sigma_0C_0YZA_0U_0T'$ is common to both bodies; the part $\Sigma_0TZ'C_0A_0Y'\Gamma'U_0$ is equivalent to the part of the representation domain with negative z values through a twofold screw rotation 2_1 around the axis $\frac{1}{4}, \frac{1}{4}, z$. Coordinates of the *points*: $\Gamma = 0,0,0 \sim \Gamma' = \frac{1}{2},\frac{1}{2},\frac{1}{2}$; $Y = 0,\frac{1}{2},0 \sim Y' = \frac{1}{2},0,\frac{1}{2}$; $Z = 0,0,\frac{1}{2} \sim Z' = \frac{1}{2},\frac{1}{2},0$; $T = \frac{1}{2},0,0 \sim T' = 0,\frac{1}{2},\frac{1}{2}$; $\Sigma_0 = \sigma_0,0,0 \sim U_0 = u_0,\frac{1}{2},\frac{1}{2}$; $A_0 = a_0,0,\frac{1}{2} \sim C_0 = c_0,\frac{1}{2},0$. The coordinates of the points are $\sigma_0 = 1/4[1 + (b^{*2} + c^{*2})/a^{*2}]$; $u_0 = 1/2 - \sigma_0$; $a_0 = 1/4[1 + (b^{*2} - c^{*2})/a^{*2}]$; $c_0 = 1/2 - a_0$. The sign $\sim$ means symmetrically equivalent. There are no special points. The points Γ, *Z*, *Y* and *T'* belong to special lines, Σ_0, U_0, A_0 and C_0 belong to special planes. The points with negative z coordinates are equivalent to those already listed. *Lines*: $\Lambda = \Gamma Z = 0,0,z$; $H = YT' = 0,\frac{1}{2},z$. The lines $\Sigma = \Gamma\Sigma_0 = x,0,0$; $U = T'U_0 = x,\frac{1}{2},\frac{1}{2}$; $A = ZA_0 = x,0,\frac{1}{2}$; $C = YC_0 = x,\frac{1}{2},0$; $\Delta = \Gamma Y = 0,y,0$; $B = ZT' = 0,y,\frac{1}{2}$; U_0A_0, $A_0\Sigma_0$, Σ_0C_0 and C_0U_0 have no special symmetry but belong to special planes. The lines $\Gamma\bar{Z}$ and $Y\bar{T}'$ of the representation domain to the points $\bar{Z}$ and $\bar{T}'$ with negative z coordinates are equivalent to lines of the asymmetric unit not belonging to the representation domain. *Planes*: $E = \Gamma YT'Z = 0,y,z$; $J = \Gamma\Sigma_0A_0Z = x,0,z$; $K = YC_0U_0T' = x,\frac{1}{2},z$. The planes x, y, 0; x, y, $\frac{1}{2}$; and $\Sigma_0C_0U_0A_0$ belong to the general position *GP*, as does the negative counterpart of $\Sigma_0C_0U_0A_0$. The planes $\Gamma\bar{Z}\bar{T}'\bar{Y}$, $\Gamma\Sigma_0\bar{A}_0\bar{Z}$ and $Y\bar{T}'\bar{U}_0C_0$ of the representation domain to the points $\bar{Z}$, $\bar{T}'$, $\bar{A}_0$ and $\bar{U}_0$ with negative z coordinates are equivalent to planes of the asymmetric unit not belonging to the representation domain. For the parameter ranges see Table 1.5.5.4.

The fourth possible type of Brillouin zone with $b^{*2} > a^{*2} + c^{*2}$ is similar to that displayed in (*c*). It can be obtained from this by exchanging $\mathbf{a}^*$ and $\mathbf{b}^*$ and changing the letters for the points, lines and planes correspondingly.

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