Acta Crystallographica Section A
Foundations and Advances
ISSN 2053-2733

Received 1 September 2013
Accepted 11 November 2013

Brillouin-zone database on the *Bilbao Crystallographic Server*[1]

Mois I. Aroyo,[a]* Danel Orobengoa,[a] Gemma de la Flor,[a] Emre S. Tasci,[b] J. Manuel Perez-Mato[a] and Hans Wondratschek[c]

[a]Departamento Física de la Materia Condensada, Universidad del País Vasco (UPV/EHU), Bilbao, Spain, [b]Physics Department, Middle East Technical University, Ankara, Turkey, and [c]Laboratorium für Applikationen der Synchrotronstrahlung (LAS), Universität Karlsruhe, Germany. Correspondence e-mail: mois.aroyo@ehu.es

The Brillouin-zone database of the *Bilbao Crystallographic Server* (http://www.cryst.ehu.es) offers **k**-vector tables and figures which form the background of a classification of the irreducible representations of all 230 space groups. The symmetry properties of the wavevectors are described by the so-called reciprocal-space groups and this classification scheme is compared with the classification of Cracknell *et al.* [*Kronecker Product Tables*, Vol. 1, *General Introduction and Tables of Irreducible Representations of Space Groups* (1979). New York: IFI/Plenum]. The compilation provides a solution to the problems of uniqueness and completeness of space-group representations by specifying the independent parameter ranges of general and special **k** vectors. Guides to the **k**-vector tables and figures explain the content and arrangement of the data. Recent improvements and modifications of the Brillouin-zone database, including new tables and figures for the trigonal, hexagonal and monoclinic space groups, are discussed in detail and illustrated by several examples.

1. Introduction

The *Bilbao Crystallographic Server* (http://www.cryst.ehu.es) is a web site offering online crystallographic programs and databases (Aroyo, Perez-Mato *et al.*, 2006; Aroyo, Kirov *et al.*, 2006; Aroyo *et al.*, 2011). The aim of this contribution is to present the Brillouin-zone database available on the server focusing on the recent modifications and improvements of the wavevector data. The database includes for all space groups Brillouin-zone figures and tables of the wavevectors that form the background of the classification of the irreducible representations of space groups. The wavevectors of reciprocal space are classified in terms of their symmetry described by the symmorphic space groups available in Volume *A* of *International Tables for Crystallography* (2002) (henceforth referred to as ITA). This is possible because of the isomorphism between the reciprocal-space groups, describing the symmetry of the wavevectors, and the symmorphic space groups in direct space (Wintgen, 1941). In the database, the ITA classification scheme is compared with the 'traditional' classification of the wavevectors available in the tables of space-group representations by Cracknell *et al.* (1979) (in the following, referred to as CDML).

The recent modifications of the database focus on a general improvement and homogenization of the stored data and a clearer presentation of the Brillouin-zone figures. The Brillouin-zone figures for trigonal, hexagonal and rhombohedral space groups are redrawn, applying a much more visual clinographic projection, that had also been used for the rest of the space groups. The figures and tables for monoclinic space groups in *unique axis b* setting have also been included in the database.

In addition, we have developed an auxiliary computer tool for the complete characterization of the wavevectors: given the wavevector coefficients referred to primitive or conventional dual bases, the program assigns the corresponding wavevector symmetry type, specifies its CDML label, determines the little co-group of the wavevector and generates the arms of the wavevector star.

Some basic concepts related to the reciprocal-space groups and their application in the classification of wavevectors are briefly reviewed in §2. Readers are referred to Aroyo & Wondratschek (1995) and to ch. 1.5 of Volume *B* of *International Tables for Crystallography* (2010) (referred to as ITB) for more details of the reciprocal-space-group approach. Short guides to the **k**-vector data displayed in the figures and tables of the Brillouin-zone database are presented in §3. The examples of §4 illustrate the new data included in the database.

[1] This article forms part of a special issue dedicated to mathematical crystallography, which will be published as a virtual special issue of the journal in 2014.

2. Classification of wavevectors

Referred to a coordinate system consisting of an origin O and a basis $\{\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3\}$, the symmetry operations of a space group $\mathcal{G}$ are described by matrix-column pairs $(\mathbf{W}, \mathbf{w})$. The (3×3) matrices $\mathbf{W}$ correspond to the linear parts of the symmetry operations while the translation parts are described by the (3×1) columns $\mathbf{w}$. The infinite set of translations $\mathbf{t}_i$ of $\mathcal{G}$ form the *translation group* $\mathcal{T}_{\mathcal{G}}$ of $\mathcal{G}$. For each translation its translation vector is defined and the set of all translation vectors of $\mathcal{T}_{\mathcal{G}}$ is called the *vector lattice* $\mathbf{L}$ of $\mathcal{G}$. The set of linear parts of the symmetry operations of $\mathcal{G}$ form a finite group which is called the *point group* $\mathcal{P}_{\mathcal{G}}$ of the space group $\mathcal{G}$, also designated by $\overline{\mathcal{G}}$ in some of the books on representation theory.

The determination, classification, labelling and tabulation of irreducible representations (irreps) of space groups are based on the use of wavevectors $\mathbf{k}$. The $\mathbf{k}$ vectors are vectors of the *reciprocal space* of $\mathcal{G}$ and can be represented as $\mathbf{k} = \sum_{i=1}^{3} k_i \mathbf{a}_i^*$ where $\{\mathbf{a}_1^*, \mathbf{a}_2^*, \mathbf{a}_3^*\}$ is the basis of the *reciprocal lattice* $\mathbf{L}^*$. The basis $\{\mathbf{a}_1^*, \mathbf{a}_2^*, \mathbf{a}_3^*\}$ is the *dual basis* of $\{\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3\}$ of $\mathbf{L}$ and its vectors $\mathbf{a}_i^*$ are defined by the relations $\mathbf{a}_i \cdot \mathbf{a}_j^* = 2\pi\delta_{ij}$, where δ_{ij} is the Kronecker symbol. The symmetry properties of the wavevectors are described by the so-called *reciprocal-space groups* $(\mathcal{G})^*$ whose elements are operations of the type $(\mathbf{W}, \mathbf{K}) = (\mathbf{I}, \mathbf{K})(\mathbf{W}, \mathbf{o})$ with $\mathbf{W} \in \overline{\mathcal{G}}$ and $\mathbf{K} \in \mathbf{L}^*$ [$\mathbf{I}$ is the (3×3) unit matrix and $\mathbf{o}$ is the (3×1) zero column]. The group $(\mathcal{G})^*$ is the semidirect product of the point group $\overline{\mathcal{G}}$ and the translation group of the reciprocal lattice $\mathbf{L}^*$ of $\mathcal{G}$.

From its definition it follows that the reciprocal-space group $(\mathcal{G})^*$ is isomorphic to a *symmorphic space group* $\mathcal{G}_0$ (for symmorphic space groups, *cf.* ITA, §8.1.6). Space groups of the same type define the same type of reciprocal-space group $(\mathcal{G})^*$. In addition, 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 $(\mathcal{G})^*$ (Wintgen, 1941) (for the definition and symbols of arithmetic crystal classes, see §8.2.3 of ITA). For about 2/3 of the space groups, $(\mathcal{G})^*$ and $\mathcal{G}$ belong to the same arithmetic crystal class, *i.e* given the space group $\mathcal{G}$, its reciprocal-space group $(\mathcal{G})^*$ is isomorphic to the symmorphic group $\mathcal{G}_0$ related to $\mathcal{G}$. However, there are a number of cases when the arithmetic crystal classes of $\mathcal{G}$ and $(\mathcal{G})^*$ are different. For example, if the lattice symbol of $\mathcal{G}$ is F or I, then the lattice symbol of $(\mathcal{G})^*$ is I or F. (The tetragonal space groups form an exception to this rule; for these the symbol I persists.) The rest of the exceptions are listed in Table 1.

To find all irreps of $\mathcal{G}$, it is necessary to consider only the wavevectors of the so-called *representation domain*. It is defined as a simply connected part of the (first) Brillouin zone (a unit cell of the reciprocal space) which contains exactly one $\mathbf{k}$ vector of each orbit of $\mathbf{k}$. One of the main difficulties in comparing the published data of irreps of space groups is due to different choices of representation domains used by different authors [see *e.g.* Table 7 in Stokes & Hatch (1988)]. The isomorphism between the reciprocal-space groups and the symmorphic space groups permits the application of crystallographic conventions in the classification of the wavevectors. For example, the unit cells of the symmorphic groups listed in ITA can replace the Brillouin zones as unit cells of the reciprocal space. The asymmetric units of space groups can serve as representation domains. The advantage of choosing the crystallographic unit cells and their asymmetric units becomes especially evident in the low-symmetry space groups where the Brillouin zones may even belong to different topological types depending on the ratios of the lattice parameters. Faces and lines on the surface of the Brillouin zone may appear or disappear or change their relative sizes depending on the lattice parameters. On the contrary, the unit cells and their asymmetric units are independent of the ratios of the lattice parameters. For that reason, Miller & Love (1967), Bradley & Cracknell (1972) and CDML replace the different complicated bodies of the Brillouin zones of the triclinic and monoclinic lattices by simple primitive unit cells of the reciprocal lattices.

Table 1
Reciprocal-space groups for the cases when the arithmetic crystal classes of $\mathcal{G}$ and $\mathcal{G}^*$ are different.

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

The action of the reciprocal-space groups $(\mathcal{G})^*$ on the wavevectors results in their distribution into orbits of *symmetry-equivalent* $\mathbf{k}$ vectors with respect to $(\mathcal{G})^*$. Thanks to the isomorphism of $(\mathcal{G})^*$ and the symmorphic space groups $\mathcal{G}_0$, the different types of $\mathbf{k}$ vectors correspond to the different kinds of point orbits (Wyckoff positions) of $\mathcal{G}_0$. In this way, a complete list of the special sites in the Brillouin zone of $(\mathcal{G})^*$ is provided by the Wyckoff positions of $\mathcal{G}_0$ found in ITA. The site symmetry of ITA corresponds to the little co-group of the wavevector; the number of arms of the star of the wavevector follows from the multiplicity of the Wyckoff position. The Wyckoff positions with 0, 1, 2 or 3 variable parameters correspond to special $\mathbf{k}$-vector points, $\mathbf{k}$-vector lines, $\mathbf{k}$-vector planes or to the set of all general $\mathbf{k}$ vectors, respectively. A $\mathbf{k}$-*vector type*, *i.e.* the set of all $\mathbf{k}$ vectors corresponding to a Wyckoff position, consists of complete orbits of $\mathbf{k}$ vectors and thus of full stars of $\mathbf{k}$ vectors. The different orbits (and stars) of a $\mathbf{k}$-vector type are obtained by varying the free parameters. Correspondingly, the irreps of $\mathbf{k}$ vectors of a $\mathbf{k}$-vector type are interrelated by parameter variation and are said to belong to the same *type of irreps* (Boyle, 1986). In this way all wavevector stars giving rise to the same type of irreps are related to the same Wyckoff position and designated by the same Wyckoff letter.

It is worth noting that being of the same $\mathbf{k}$-vector type is only a necessary but not a sufficient condition for $\mathbf{k}$-vector equivalence: two wavevectors $\mathbf{k}_1$ and $\mathbf{k}_2$ are called *equivalent* if they belong to the same orbit of $\mathbf{k}$ vectors, *i.e.* if there exists $\mathbf{W} \in \overline{\mathcal{G}}$ and $\mathbf{K} \in \mathbf{L}^*$ such that $\mathbf{k}_2 = \mathbf{k}_1\mathbf{W} + \mathbf{K}$.

A complete set of irreps of $\mathcal{G}$ is derived by considering exactly one **k**-vector representative per **k**-vector orbit. To achieve that it is necessary to specify the exact parameter ranges of the independent **k**-vector regions within the asymmetric unit or the representation domain. However, such data are not available in the literature. One of the aims of the Brillouin-zone database of the *Bilbao Crystallographic Server* is to provide a solution to the problems of uniqueness and completeness of space-group irreps by listing the exact parameter ranges for general and special **k** vectors. For this purpose it is advantageous to describe the different **k**-vector stars belonging to a Wyckoff position applying the so-called *uni-arm* description. Two **k** vectors of a Wyckoff position are called *uni-arm* if one can be obtained from the other by parameter variation. The description of **k**-vector stars of a Wyckoff position is called *uni-arm* if the **k** vectors representing these stars are uni-arm. Frequently, in order to achieve uni-arm description, it is necessary to transform **k** vectors to equivalent ones. In addition, to enable a uni-arm description, symmetry lines outside the asymmetric unit may be selected as orbit representatives. Such a segment of a line is called a *flagpole*. In analogy to the flagpoles, symmetry planes outside the asymmetric unit may be selected as orbit representatives. Such a segment of a plane is called a *wing*.

For details on the procedure for the determination of the independent ranges of the **k**-vector regions of the asymmetric units, the reader is referred to ch. 1.5 of ITB. The monoclinic example in §4 illustrates the utility of the uni-arm description in the analysis of the **k**-vector parameter ranges.

3. Brillouin-zone database

The **k**-vector data of the Brillouin-zone database of the *Bilbao Crystallographic Server* are accessed by the retrieval tool *KVEC* (http://www.cryst.ehu.es/cryst/get_kvec.html) which uses as input the ITA number of the space group. The output consists essentially of wavevector tables and figures. There are several sets of figures and tables for the same space group when its Brillouin-zone shape depends on the lattice parameters of the reciprocal lattice. The **k**-vector data are the same for space groups of the same arithmetic crystal class.

In the **k**-vector tables, the wavevector data of CDML are compared with the Wyckoff-position data of ITA. Each **k**-vector type is specified by its label and coefficients as listed in CDML. The corresponding Wyckoff positions are described by Wyckoff letters, multiplicities and site-symmetry groups. The parameter descriptions specify the independent parameter ranges chosen in such a way that each orbit of the Wyckoff positions of ITA, *i.e.* each **k**-vector orbit, is also listed *exactly once*. In the figures, the Brillouin zones of CDML and the conventional unit cells of ITA are displayed. The asymmetric units play the role of the representation domains of the Brillouin zones and they are chosen often in analogy to those of ITA.

3.1. Guide to the k-vector tables

Each **k**-vector table is headed by the corresponding Hermann–Mauguin symbol of the space group, its ITA number and the symbol of the arithmetic crystal class to which the space group belongs. If there is more than one table for an arithmetic crystal class, then these tables refer to different geometric conditions for the lattice parameters that are indicated after the symbol of the arithmetic crystal class. For example, the conditions '$\sqrt{3}a < \sqrt{2}c$' or '$\sqrt{3}a > \sqrt{2}c$' distinguish the two topologically different Brillouin zones for the rhombohedral space groups, see *e.g.* Table 5 and Figs. 3 and 4. The space groups of the arithmetic crystal class are also indicated in the headline block. They are followed by the symbol of the reciprocal-space-group type [*e.g.* '$(R3)^*$, No. 146' for the arithmetic crystal class $3R$ in Table 5] together with the conditions for the lattice parameters of the reciprocal lattice, if any. From the **k**-vector table there is a link to the corresponding Brillouin-zone figure.

Each table consists of two main parts. The first two columns under the heading '**k**-vector description' refer to the description of **k** vectors found in Tables 3.9 and 3.11 of CDML. It consists of labels of **k** vectors (column 1) and their parameter descriptions (column 2). (Note that CDML substitute the Greek-character labels for the symmetry points and lines inside the Brillouin zone by a symbol consisting of two Roman characters, *e.g.* *GM* for Γ, *LD* for Λ *etc.*) No ranges for the parameters are listed in CDML. Apart from the labels of points, lines and planes of CDML which are retained in the listings of the Brillouin-zone database, many new names have been given to points and lines which are not listed in CDML. In such cases, lines equivalent, for example, to a line H or the end points of a line H, as well as points equivalent to a point H may also be designated by the letter H but distinguished by indices. In order to recognize points and lines easily, the indices of points are always even: H_0, H_2, H_4; those of lines are always odd: H_1, H_3. The new **k** vectors are equivalent to those of CDML and are necessary to enable the uni-arm description of the **k**-vector types. The sign '$\sim$' relates equivalent **k** vectors, see *e.g.* the lines $S \sim S_1 = [HL_0]$ in Table 4 and Fig. 2, or the line $P \sim P_1 = [P_0T]$ and the point $T \sim T_2$ in Table 5 and Fig. 3.

Different **k** vectors with the *same* CDML label always belong to the same **k**-vector type, *i.e.* they correspond to the same Wyckoff position. **k** Vectors with *different* CDML labels may either belong to the same or to different types of **k** vectors. When **k** vectors with different CDML labels belong to the same **k** type, the corresponding parameter descriptions are followed by the letters 'ex' (from Latin, with the meaning of 'out of' or 'from'). Symmetry points, lines of symmetry or planes of CDML, related to the same Wyckoff position, are grouped together in a block. In the **k**-vector tables, neighbouring Wyckoff-position blocks are distinguished by a slight difference in the background colour. For example, the **k** vectors of $R3$ (Table 5) are distributed in two **k**-vector types: (i) the Wyckoff-position block $3a$ formed by special wavevectors of a **k**-vector line along a threefold axis, and (ii)

Table 2
'Conventional' **k**-vector coefficients k_j (*i.e.* with respect to a basis dual to the conventional basis of ITA) expressed by the 'primitive' **k**-vector coefficients k_{pj} (*i.e.* referred to a primitive basis) for the different Bravais types of lattices in direct space.

Lattice types	k_1	k_2	k_3
$aP, mP, oP, tP, cP, hP, rP$	k_{p1}	k_{p2}	k_{p3}
mA, oA	k_{p1}	$k_{p2}-k_{p3}$	$k_{p2}+k_{p3}$
mC, oC	$k_{p1}+k_{p2}$	$-k_{p1}+k_{p2}$	k_{p3}
oF, cF	$-k_{p1}+k_{p2}+k_{p3}$	$k_{p1}-k_{p2}+k_{p3}$	$k_{p1}+k_{p2}-k_{p3}$
oI, cI, tI	$k_{p2}+k_{p3}$	$k_{p1}+k_{p3}$	$k_{p1}+k_{p2}$
hR (hexagonal)	$k_{p1}-k_{p2}$	$k_{p2}-k_{p3}$	$k_{p1}+k_{p2}+k_{p3}$

Table 3
'Conventional' **k**-vector coefficients k_j (*i.e.* with respect to a basis dual to the conventional basis of ITA) expressed by the 'ITA' **k**-vector coefficients k_{aj} (*i.e.* referred to the conventional ITA basis of $\mathcal{G}_0$) 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)	$2k_{a1}-k_{a2}$	$-k_{a1}+2k_{a2}$	$3k_{a3}$

general **k** vectors corresponding to the general-position block 9*b* of *R*3. The parameter description of the uni-arm region of a **k**-vector type is shown in the last row of the corresponding Wyckoff-position block.

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

The wavevector coefficients of CDML (column 2 of the **k**-vector tables) refer always to a primitive basis irrespective of whether the conventional description of the space group in ITA is with respect to a centred or primitive basis. For that reason, for space groups with centred lattices, the wavevector coefficients with respect to the usual conventional reciprocal basis, *i.e.* dual to the conventional centred basis in direct space of ITA, are also listed in the column under the heading 'Conventional basis' of the **k**-vector tables. The relations between the 'conventional' $(k_1,\ k_2,\ k_3)$ and 'primitive' coefficients $(k_{p1},\ k_{p2},\ k_{p3})$ of the wavevectors are summarized in Table 2. For example, a **k**-vector point of an *LD* line of *R*3 (Table 5) with primitive coefficients $(\frac{1}{4},\frac{1}{4},\frac{1}{4})$ is described as $(0,0,\frac{3}{4})$ with respect to a basis dual to the conventional hexagonal setting of *R*3. For space groups with primitive lattices, the wavevector coefficients referred to a primitive basis coincide with those referred to the basis dual to the conventional one of ITA.

The data for the crystallographic classification scheme of the wavevectors are listed under the heading 'ITA description' in the **k**-vector tables. The columns 'Wyckoff positions' show the data of 'multiplicity', 'Wyckoff letter' and 'site symmetry' of the Wyckoff positions of the symmorphic space group $\mathcal{G}_0$ of ITA which is isomorphic to the reciprocal-space group $(\mathcal{G})^*$. The multiplicity of a Wyckoff position divided by the number of lattice points in the conventional unit cell of ITA equals the number of arms of the star of the **k** vector of the Wyckoff-position block. The alphabetical sequence of the Wyckoff positions determines the sequence of the CDML labels. The tables start with the Wyckoff letter *a* for the Wyckoff position of the highest site symmetry and proceed in alphabetical order until the *general position* (*GP*) is reached. 'Oriented' point-group symbols are used to indicate the site-symmetry groups which coincide with the little co-groups of the wavevectors (for 'oriented' point-group symbols *cf.* ITA, §2.2.12). The *parameter description* of the Wyckoff position of $\mathcal{G}_0$ is shown in the last column of the wavevector tables. It consists of a coordinate triplet of a representative point of the Wyckoff position and algebraic statements for the description of the parameter ranges. Because of the isomorphism between $\mathcal{G}_0$ and $(\mathcal{G})^*$ the coordinate triplets of the Wyckoff positions of $\mathcal{G}_0$ can be interpreted as **k**-vector coefficients $(k_{a1},\ k_{a2},\ k_{a3})$ determined with respect to the conventional ITA basis of $\mathcal{G}_0$. The relation between the 'ITA' coefficients $(k_{a1},\ k_{a2},\ k_{a3})$ and the 'conventional' coefficients $(k_1,\ k_2,\ k_3)$ is shown in Table 3. (For more details on the relationships between the different sets of **k**-vector coefficients, the reader is referred to ch. 1.5 of ITB where the 'ITA' coefficients are denoted as *adjusted* coefficients.) As an example consider the line *DT* of *P*321 (Table 4 and Fig. 2). According to the ITA description, it corresponds to the Wyckoff position 2*g* with a site-symmetry group 3... Its parameter description $0, 0, z$: $0 < z < \frac{1}{2}$ indicates that the independent segment of the line $0, 0, z$ is limited by the special **k**-vector points $\Gamma\,(z=0)$ and $A\,(z=\frac{1}{2})$ with z varying between 0 and $\frac{1}{2}$. In some cases, the algebraic expressions are substituted by the designation of the parameter region in order to avoid clumsy notation. The parameter descriptions of the flagpoles and the wings are shown under the **k**-vector tables.

Because of the dependence of the shape of the Brillouin zone on the lattice parameter relations there may be vertices of the Brillouin zone with a variable coordinate. If such a point is displayed and designated in the tables and figures by an upper-case letter, then the label of its variable coefficient used in the parameter-range descriptions is the same letter but lower case. Thus, the variable coefficent of the point G_0 is g_0, of LD_0 is ld_0 *etc.* (*cf.* Table 5).

As already indicated, the *parameter ranges* are chosen such that each orbit of the Wyckoff position of ITA, *i.e.* also each **k**-vector orbit, is listed exactly once. As a result, one usually gets rather complicated descriptions of the independent parameter regions included in the *general-position* block. For example, the statement found in Table 4

$$
\begin{aligned}
GP\;\; u, v, w\;\; 6\;\; l\;\; 1\;\; & x, y, z : -x < y < \tfrac{x}{2}, 2x - 1 < y, -\tfrac{1}{2} < z \le \tfrac{1}{2} \cup \\
& \cup\; x, -x, z : 0 < x < \tfrac{1}{3}, 0 < z < \tfrac{1}{2} \cup \\
& \cup\; x, \tfrac{x}{2}, z : 0 < x < \tfrac{2}{3}, 0 < z < \tfrac{1}{2} \cup \\
& \cup\; x, 2x - 1, z : \tfrac{1}{3} < x < \tfrac{2}{3}, 0 < z < \tfrac{1}{2}
\end{aligned}
$$

means that the description of the asymmetric unit is split into a three-dimensional set (body) and three two-dimensional sets (planes). Apart from the points inside the body, the three-dimensional set includes the points of one of its boundary planes, namely the plane at $z = \frac{1}{2}$. Together the regions contain exactly one representative for each **k**-vector orbit of the *general position* (*GP*) of the reciprocal-space group.

At the bottom of the web page with the **k**-vector table one finds an auxiliary tool which allows the complete characterization of any wavevector of the reciprocal space (not restricted to the first Brillouin zone): given the **k**-vector coefficients referred either to a primitive (CDML) or to a conventional basis, the program assigns the **k** vector to the corresponding wavevector symmetry type, specifies its CDML label, and calculates the little co-group and the arms of the **k**-vector stars. Consider, for example, a **k** vector with coefficients (0.4, 1.3, 0) of the space group $P321$ (No. 150), *cf.* Table 4 and Fig. 2. It is a vector outside the Brillouin zone and its coefficients do not correspond to any of the parameter descriptions of the **k**-vector representatives listed in Table 4. The output of the auxiliary tool indicates that **k** (0.4, 1.3, 0) is a point of a special **k**-vector line of type *LD* and belongs to the Wyckoff-position block 3*j*. Its star consists of three **k** vectors, $\mathbf{k}^* = \{(0.4, 1.3, 0), (1.3, -1.7, 0), (-1.7, 0.4, 0)\}$. The little co-group ..2 is generated by a twofold rotation that can be identified by direct inspection among the symmetry operations of $(P312)^*$ as $2x, 0, 0\,(x - y, \bar{y}, \bar{z})$.

3.2. Guide to the figures

As for the tables, the headline blockfor each figure includes the specification of the space group, its arithmetic crystal class and all space groups that belong to that arithmetic crystal class. Different figures for the same arithmetic crystal class are distinguished by the corresponding geometric conditions for the lattice. The corresponding conditions for the lattice parameters of the reciprocal lattice are indicated after the symbol of the reciprocal-space group.

The Brillouin zones are projected onto the drawing plane by a clinographic projection (see *e.g.* Smith, 1982). The coordinate axes are designated by k_x, k_y and k_z; the k_z-coordinate axis points upward in the projection plane. The diagrams of the Brillouin zones follow those of CDML in order to facilitate comparison of the data. The origin O with coefficients (0, 0, 0) always coincides with the centre of the Brillouin zone and is called Γ (indicated as *GM* in the **k**-vector tables).

In the Brillouin-zone figures the representation domains of CDML are compared with the asymmetric units of ITA. If the primitive basis of CDML $\{\mathbf{g}_1, \mathbf{g}_2, \mathbf{g}_3\}$ and the ITA basis $\{\mathbf{k}_x, \mathbf{k}_y, \mathbf{k}_z\}$ do not coincide, then their relations are indicated below the Brillouin-zone figures. A statement of whether the representation domain of CDML and the asymmetric unit are identical or not is given below the **k**-vector table. The asymmetric units are often *not* fully contained in the Brillouin zone but protrude from it, in particular by *flagpoles* and *wings*.

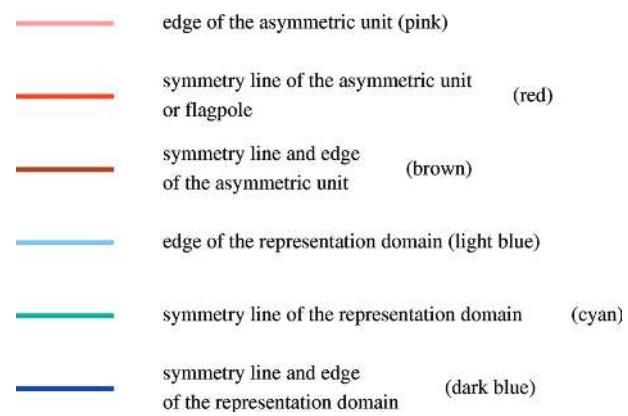

Figure 1
Colour coding of the different lines applied in the Brillouin-zone diagrams.

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

The representatives of the orbits of **k**-vector symmetry points or of symmetry lines, as well as the edges of the representation domains of CDML and of the asymmetric units are brought out in colour:

(*a*) *Symmetry points*. A representative point of each orbit of symmetry points is designated by a red or cyan filling of the circle with its label also in red or cyan if it belongs to the asymmetric unit or to the representation domain of CDML. If both colours could be used, *e.g.* if the asymmetric unit coincides with the representation domain, the colour is red. Note that a point is coloured red or cyan only if it is really a symmetry *point*, *i.e.* its little co-group is a proper supergroup of the little co-groups of all points in its neighbourhood. Points listed by CDML are not coloured if they are part of a symmetry line or symmetry plane only.

(*b*) *Symmetry lines*. Coloured lines are drawn as solid if they are 'visible', *i.e.* if they are not hidden by the Brillouin zone or by the asymmetric unit. A hidden symmetry line or edge of the asymmetric unit is not suppressed but is shown as a *dashed line*. The colour coding of the different lines applied in the Brillouin-zone diagrams is displayed in Fig. 1.

The labels of the special lines shown on the Brillouin-zone figures are always red or cyan irrespective of whether the lines are edges of the representation domain or not. Common edges of an asymmetric unit and a representation domain are coloured pink if they are not symmetry lines simultaneously.

Flagpoles are always coloured red – see *e.g.* the line P_1 or PA_1 in Fig. 3. Symmetry planes are not distinguished in the figures. However, wings are indicated in the figures and they are always coloured pink – see *e.g.* Figs. 5 and 6.

4. Examples

The relation between the traditional and the reciprocal-space-group descriptions of the wavevector types is illustrated by the following examples. They are chosen among the new tables and figures of the Brillouin-zone database developed for space groups of the hexagonal P lattice, rhombohedral space groups and monoclinic space groups in *unique axis b* setting. The figures and tables included here form part of the output of the access tool *KVEC*.

4.1. k-Vector table and Brillouin zone for space group *P*321 (No. 150)

The new data for space groups of the hexagonal P lattice are illustrated by the **k**-vector table shown in Table 4 and the Brillouin-zone diagram of the space group $P321$ (No. 150) shown in Fig. 2. The reciprocal lattice of a hexagonal P lattice is also a hexagonal P lattice and the Brillouin zone is a hexagonal prism with z extending in the range $(-1/2, 1/2]$, *i.e* $-\frac{1}{2} < z \le \frac{1}{2}$. The conventional basis for the reciprocal lattice has $\gamma^* = 60^\circ$ while the ITA description of hexagonal space groups is based on 120° $(\mathbf{a}_H, \mathbf{b}_H)$ basis. In the Brillouin-zone diagrams, the axes $\mathbf{k}_x, \mathbf{k}_z$ are taken along $\mathbf{a}_H, \mathbf{c}_H$ while $\mathbf{k}_y$ points out in the direction of $\mathbf{a}_H + \mathbf{b}_H$. The table and diagram of $P321$ can also be used for the space groups $P3_121$ (No. 152) and $P3_221$ (No. 154) which belong to the arithmetic crystal class $321P$. As the asymmetric unit and the representation domain coincide, the basic colour of their edges is pink. Note that the reciprocal-space group of $321P$ is $(P312)^*$ (*cf.* Table 1).

The list of the special **k** vectors includes special points of symmetry and special lines of symmetry. The points A, H, HA, Γ, K and KA are represented by red circles as they are special **k**-vector points of symmetry 32 (*cf.* Table 4). The lines DT (indicated as Δ on Fig. 2), P and PA are brown because they correspond to each of the three tertiary axes of the asymmetric unit and at the same time form its edges. The special **k**-vector lines T, TA and LE are coloured cyan as they do not form part of the edges of the representation domain. Together with the line LD (represented as Λ in Fig. 2) and the point M, they belong to the Wyckoff-position block $3j$, *i.e.* all these different wavevectors belong to the same **k**-vector type. Its uni-arm description is achieved by the definition of two flagpoles, stretching out of the asymmetric unit along the Λ line. The flagpole LE_1 is equivalent to LE, while the flagpole $T_1 \cup M_0 \cup TA_1$ substitutes $T \cup M \cup TA$. The uni-arm description of the **k**-vector type $3j$ is shown in the last row of the Wyckoff-position block. The parameter description of the flagpoles and their parameter ranges with respect to the basis of the reciprocal-space group are given below the **k**-vector table.

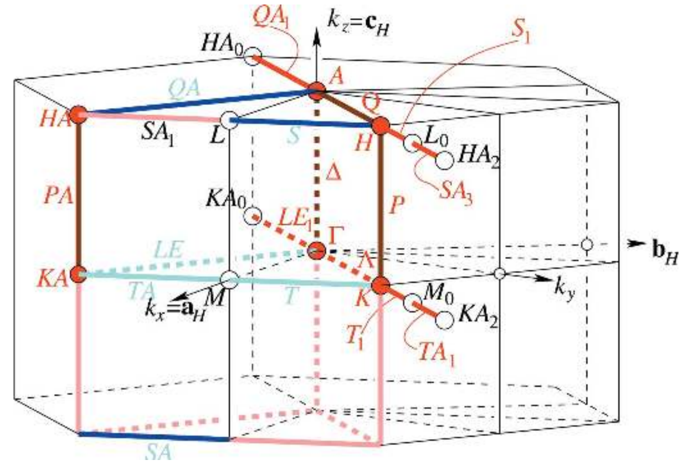

Figure 2
Brillouin zone, asymmetric unit and representation domain of CDML of the arithmetic crystal class $321P$: space groups $P321$ (No. 150), $P3_121$ (No. 152) and $P3_221$ (No. 154); reciprocal-space group $(P312)^*$. The representation domain of CDML coincides with the asymmetric unit.

The **k**-vector lines S, QA and SA are dark blue as they are selected in CDML to represent the special twofold symmetry lines along the edges of the representation domain. Together with the line Q and the point L, they belong to the special **k**-vector type of the Wyckoff-position block $3k$. As in the case of the $3j$ type, a uni-arm description can be achieved by defining two flagpoles stretching out of the representation domain along the **k**-vector line Q.

It has already been pointed out that special **k**-vector points and lines are brought out in colours only if they are chosen as orbit representatives of the corresponding **k**-vector type. For example, although SA_1 is along a binary axis, it is not coloured as a special line (the pink colour indicates an asymmetric unit edge) since it is not chosen as an orbit representative in any of the two descriptions: SA_1 is substituted by SA in the CDML description or by SA_3 in the case of the uni-arm description. Likewise, the points KA_2 and KA_0 (of symmetry 32) are not coloured as special points as they belong to the orbit of the special **k**-vector point KA, chosen as an orbit representative and shown in the diagram by a circle filled in red. [The fact that the three points belong to the same **k**-vector orbit is evident from their coefficients: $KA\,(\frac{2}{3}, -\frac{1}{3}, 0)$, $KA_2\,(\frac{2}{3}, \frac{2}{3}, 0)$, $KA_0\,(-\frac{1}{3}, -\frac{1}{3}, 0)$.]

The points L and M are examples of **k**-vector points whose little co-groups are not proper supergroups of the little co-groups of all points in their neighbourhood. In fact, although L and M are explicitly listed by CDML as special **k**-vector points, they form part of the lines S and T and in the diagram they are represented by black circles filled in with white.

4.2. Brillouin-zone diagrams of the space group *R*3 (No. 146)

The 'rhombohedral' space groups, *i.e.* space groups with a rhombohedral lattice, belong to the trigonal crystal system of ITA. Depending on the rhombohedral angle α (or the relation between the lattice parameters a and c), two topologically different Brillouin zones are to be distinguished: (i) in the

Table 4
k-Vector table for the space groups of the arithmetic crystal class 321*P* as it is shown on the *Bilbao Crystallographic Server*.

The Brillouin-zone diagram is shown in Fig. 2.

The k-vector types of space group $P321$ (150)

(Table for arithmetic crystal class 321P)

P321 - D_3^2 (150), P3$_1$21 - D_3^4 (152), P3$_2$21 - D_3^6 (154)

Reciprocal space group (P312)*, No. 149

k-vector description		ITA description			
CDML		Wyckoff position			Coordinates
Label	Coefficients				
GM	0,0,0	1	a	3.2	0,0,0
A	0,0,1/2	1	b	3.2	0,0,1/2
KA	2/3,-1/3,0	1	c	3.2	1/3,-1/3,0
HA	2/3,-1/3,1/2	1	d	3.2	1/3,-1/3,1/2
K	1/3,1/3,0	1	e	3.2	2/3,1/3,0
H	1/3,1/3,1/2	1	f	3.2	2/3,1/3,1/2
DT	0,0,u	2	g	3..	0,0,z: 0<z<1/2
PA	2/3,-1/3,u	2	h	3..	1/3,-1/3,z: 0<z<1/2
P	1/3,1/3,u	2	i	3..	2/3,1/3,z: 0<z<1/2
M	1/2,0,0 ex	3	j	..2	1/2,0,0
M ~ M$_0$		3	j	..2	1,1/2,0
LD	u,u,0 ex	3	j	..2	x,x/2,0: 0<x<2/3
LE	2u,-u,0 ex	3	j	..2	x,-x,0: 0<x<1/3
LE ~ LE$_1$		3	j	..2	x,x/2,0: -2/3<x<0
T	1/2-u,2u,0 ex	3	j	..2	1/2+x,2x,0: 0<x<1/6
T ~ T$_1$ =[K M$_0$]		3	j	..2	x,x/2,0: 2/3<x<1
TA	1/2+u,-2u,0 ex	3	j	..2	1/2-x,-2x,0: 0<x<1/6
TA ~ TA$_1$ = [M$_0$ KA$_2$]		3	j	..2	x,x/2,0: 1<x< 4/3
M$_0$+LE$_1$+LD+T$_1$+TA$_1$=[KA$_0$ KA$_2$] \ [GM, K]		3	j	..2	x,x/2,0: -2/3<x<4/3, x $\neq$ 0, 2/3
L	1/2,0,1/2 ex	3	k	..2	1/2,0,1/2
L~L$_0$		3	k	..2	1,1/2,1/2
Q	u,u,1/2 ex	3	k	..2	x,x/2,1/2: 0<x<2/3
QA	2u,-u,1/2 ex	3	k	..2	x,-x,1/2: 0<x<1/3
QA~QA$_1$ = [HA$_0$A]		3	k	..2	x,x/2,1/2: -2/3<x<0
S	1/2-u,2u,1/2 ex	3	k	..2	1/2+x, 2x,1/2: 0<x<1/6
S~S$_1$ = [H L$_0$]		3	k	..2	x,x/2,1/2: 2/3 <x<1
SA	1/2+u,-2u,-1/2 ex	3	k	..2	1/2-x,-2x,-1/2 : 0<x<1/6
SA~SA$_1$ = [L HA]		3	k	..2	1/2-x, -2x,1/2 : 0<x< 1/6
SA$_3$ ~SA$_1$ = [L$_0$ HA$_2$]		3	k	..2	x,x/2,1/2: 1<x<4/3
L$_0$+QA$_1$+Q+S$_1$+SA$_3$ = [HA$_0$ HA$_2$]\[A,H]		3	k	..2	x,x/2,1/2: -2/3<x<4/3, x $\neq$ 0, 2/3
GP	u,v,w	6	l	1	x,y,z: -x<y<x/2, 2x-1<y,-1/2<z $\leq$ 1/2 U U x,-x,z: 0<x<1/3, 0<z<1/2 U U x,x/2,z: 0<x<2/3, 0<z<1/2 U U x,2x-1,z: 1/3<x<2/3, 0<z<1/2

The representation domain of CDML is identical with the asymmetric unit.

Flagpoles: [K KA$_2$] x,x/2,0: 2/3<x<4/3

[KA$_0$ GM] x,x/2,0: -2/3<x<0

[H HA$_2$] x,x/2,1/2: 2/3<x<4/3

[HA$_0$ A] x,x/2,1/2: -2/3<x<0

acute case, with $\alpha < 90^\circ$ (or $\sqrt{3}a > \sqrt{2}c$), the Brillouin zone has 14 apices and 12 faces (it consists of the rhombohedral forms {100} and {$1\bar{1}0$} and can be called a rhombohedrally truncated distorted cube), and (ii) in the *obtuse* case with $\alpha > 90^\circ$ (or $\sqrt{3}a < \sqrt{2}c$), the Brillouin zone has 24 apices and 14 faces (it is a kind of a rhombohedrally distorted cube-octahedron and consists of deformed cubic forms {100} and {111}).

In the following, the Brillouin-zone diagrams of the space group *R*3, the simplest of the rhombohedral space groups, are considered as an example. The *R*3 diagrams of the *Bilbao Crystallographic Server* are shown in Figs. 3 and 4. While the

Table 5
k-Vector tables of the space group *R*3 (No. 146), *acute* ($\sqrt{3}a > \sqrt{2}c$) and *obtuse* ($\sqrt{3}a < \sqrt{2}c$) cases, as shown on the *Bilbao Crystallographic Server*. The Brillouin-zone diagrams are shown in Figs. 3 and 4.

The k-vector types of space group *R*3 (146)

(Table for arithmetic crystal class 3R: sqrt3a > sqrt2c)

R3 - C_3^4 (146)

Reciprocal space group (R3)*, No. 146: c*/a* > sqrt2/2

k-vector description			ITA description			
CDML		Conventional basis	Wyckoff position			Coordinates
Label	Primitive basis					
GM	0,0,0 ex	0,0,0	3	a	3.	0,0,0
T	1/2,1/2,-1/2 ex	0,1,1/2	3	a	3.	1/3, -1/3, 1/6
T~T_2			3	a	3.	0,0,1/2
LD = [GM P_2]	u,u,u ex	0,0,3u	3	a	3.	0,0,z: 0<z≤ld_0
LE = [GM R_2]	-u,-u,-u ex	0,0,-3u	3	a	3.	0,0,z: ld_0 ≤z<0
P = [P_0 T]	1/3+u,1/3+u,-2/3+u ex	0,1,3u	3	a	3.	1/3,-1/3,z: 1/2-ld_0=p_0<z<1/6
P~P_1 = [P_2 T_2]			3	a	3.	0,0,z: ld_0<z<1/2
PA = [R_0 T_4]	-1/3-u,2/3-u,-1/3-u ex	-1,1,-3u	3	a	3.	2/3,1/3,z: -1/6<z<-p_0
PA~PA_1 = [R_2 T_6]			3	a	3.	0,0,z: -1/2<z<-ld_0
GM+T_2+P_1+LD+LE+PA_1 = [T_6 T_2]			3	a	3.	0,0,z: -1/2<z≤1/2
GP	u,v,w	-v+u,-w+v,w+v+u	9	b	1	x,y,z: -x≤y≤1-x; 2x-1<y<2x; -1/6<z≤1/6

The representation domain of CDML is different from the asymmetric unit

Flagpoles: 0,0,z: 1/6<z≤1/2

0,0,z: -1/2<z<-1/6

(Table for arithmetic crystal class 3R: sqrt3a < sqrt2c)

R3 - C_3^4 (146)

Reciprocal space group (R3)*, No. 146: c*/a* < sqrt2/2

k-vector description			ITA description			
CDML		Conventional basis	Wyckoff position			Coordinates
Label	Primitive basis					
GM	0,0,0 ex	0,0,0	3	a	3.	0,0,0
T	1/2,1/2,1/2 ex	0,0,3/2	3	a	3.	0,0,1/2
LD	u,u,u ex	0,0,3u	3	a	3.	0,0,z: 0<z<1/2
LE	-u,-u,-u ex	0,0,-3u	3	a	3.	0,0,z: -1/2<z<0
GM+T+LD+LE = [T T_0]			3	a	3.	0,0,z: -1/2<z≤1/2
GP	u,v,w	-v+u,-w+v,w+v+u	9	b	1	x,y,z -x≤y≤1-x; 2x-1<y<2x; -1/6<z≤1/6

The representation domain of CDML is different from the asymmetric unit

Flagpoles: 0,0,z: 1/6<z≤1/2

0,0,z: -1/2<z<-1/6

representation domains of the acute and obtuse unit cells are of a rather complicated form, the asymmetric units in both cases have a topologically identical and relatively simple shape: it is a rhombus with an angle of 120° in the *xy* plane (a union of two equilateral triangles) with z extending from $-\frac{1}{6}$ to $\frac{1}{6}$.

In the diagrams one can distinguish a single special **k**-vector type: it is a symmetry **k**-vector line along the threefold axis. In the obtuse case, the correspondence between the CDML description of the special **k**-vector line and the uni-arm description is straightforward as the necessary segment of the line $0, 0, z$ lies entirely inside the Brillouin zone (*cf.* Table 5 and Fig. 4): the uni-arm description of the Wyckoff-position block $3a$ unifies the lines Λ and LE, and the two points Γ and T. In the hexagonal basis, it is described by the segment of the line $0, 0, z$ with z varying in the range $(-\frac{1}{2}, \frac{1}{2}]$. It is worth noting that, although listed separately in CDML, the points Γ and T obviously belong to the same **k**-vector type as the lines Λ and LE, *i.e.* the points have the same symmetry as the points on the line and, as such, they are represented by black circles filled in with white on the diagrams.

Because of the special shape of the Brillouin zone and the representation domain for the *acute* case ($\sqrt{3}a > \sqrt{2}c$), the special **k**-vector line corresponding to the Wyckoff-position block $3a$ splits into several segments: the lines Λ and LE, located inside the Brillouin zone, and the lines P and PA (coloured dark blue) at the border of the Brillouin zone (*cf.* Table 5 and Fig. 3). For the description of the end points of the segments it is necessary to introduce additional parameters as p_0 and ld_0 whose values depend on the specific relations between the lattice parameters. To enable uni-arm description, symmetry lines equivalent to P and PA, located outside the Brillouin zone and along $(0, 0, z)$, are to be selected as orbit representatives. The uni-arm description of the special **k**-vector line is formed by the union of the lines Λ and LE, the flagpoles $P_1\,(\sim P)$ and $PA_1\,(\sim PA)$, and the points Γ and $T_2\,(\sim T)$. Its parameter description $(0, 0, z)$ with z varying in the range $(-\frac{1}{2}, \frac{1}{2}]$ coincides with that of the obtuse case.

4.3. Diagrams of monoclinic groups

For monoclinic space groups, because of the variety of possible axial relations between the lattice parameters, several topologically different Brillouin zones are necessary for the classification of the wavevectors. In CDML the Brillouin zones are replaced by primitive unit cells which are always parallelepipeds independently of the axial ratios. The description of the **k**-vector types of the monoclinic space groups applied in CDML is only with respect to *unique axis c* setting and no data are available for monoclinic space groups described with respect to *unique axis b* setting. To complete the database, **k**-vector tables and figures have been generated for all six monoclinic arithmetic crystal classes: $121P$, $121C$, $1m1P$, $1m1C$, $12/m1P$ and $12/m1C$. The derivation of the new data is illustrated by the **k**-vector table and figure of $12/m1C$ shown in Table 6 and Fig. 5. For comparison, the corresponding *unique axis c* data of the arithmetic crystal class $112/mA$ are shown in Table 7 and Fig. 6.

In ITA the monoclinic space group $C2/c$ (No. 15) is described in six settings: depending on the cell choices, there are three descriptions for each of the *unique axis b* and *unique axis c* settings. The Brillouin-zone database contains **k**-vector tables and figures of two settings of $C2/c$, namely, the settings $A112/a$ (*unique axis c*, cell choice 1) and $C12/c1$ (*unique axis b*, cell choice 1). The space group $C2/c$ belongs to the arithmetic crystal class $2/mC$ which also includes the space group $C2/m$ (No. 12). In the following, we discuss briefly the **k**-vector table and figure of $A112/a$, and then proceed with the derivation of the data of $C12/c1$ from those of $A112/a$.

The reciprocal-space group of $A112/a$ is isomorphic to the symmorphic space group $A112/m$, *i.e.* the list of special Wyckoff positions of $A112/m$ indicates the special **k**-vector types of $A112/a$. In fact, the Wyckoff-position data, including multiplicities, Wyckoff letters, site-symmetry groups and coordinate triplets of Table 7 are taken directly from ITA. For the determination of the parameter ranges one starts by

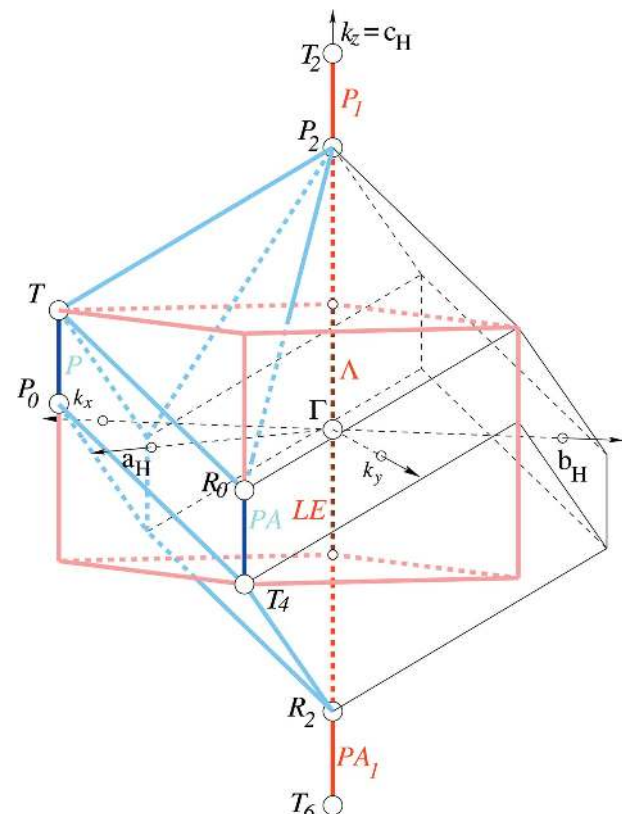

Figure 3
Brillouin zone, asymmetric unit and representation domain of CDML for the space group $R3$ (No. 146): *acute* case ($\sqrt{3}a > \sqrt{2}c$); reciprocal-space group $(R3)^*$. The representation domain of CDML is different from the asymmetric unit.

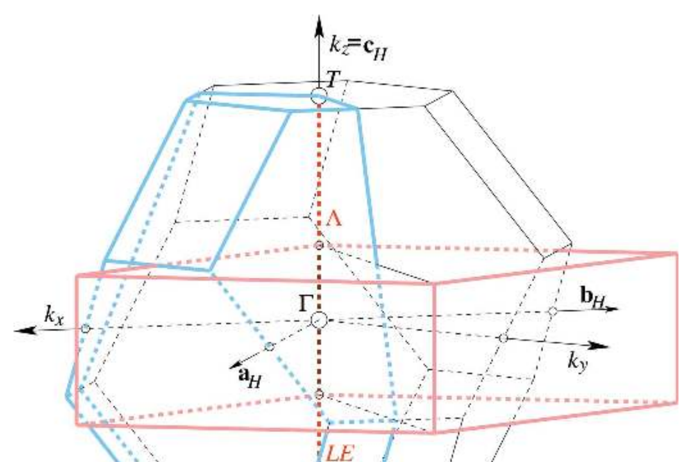

Figure 4
Brillouin zone, asymmetric unit and representation domain of CDML for the space group $R3$ (No. 146): *obtuse* case ($\sqrt{3}a < \sqrt{2}c$); reciprocal-space group $(R3)^*$. The representation domain of CDML is different from the asymmetric unit.

Table 6
k-Vector table of the space groups of the arithmetic crystal class $12/m1C$ ($2/mC$) as shown on the *Bilbao Crystallographic Server*.

The unit-cell diagram is shown in Fig. 5.

The k-vector types of space group $C2/c$ (15) [unique axis b]

(Table for arithmetic crystal class 2/mC)

C12/m1(C2/m) - C_{2h}^3 (12), C12/c1(C2/c) - C_{2h}^6 (15)

Reciprocal space group (C12/m1)*, No. 12

k-vector description			ITA description			
Label	Primitive basis	Conventional basis	Wyckoff Position			Coordinates
GM	0,0,0	0,0,0	2	a	2/m	0,0,0
Y	1/2,1/2,0	0,1,0	2	b	2/m	0,1/2,0
A	0,0,1/2	0,0,1/2	2	c	2/m	0,0,1/2
M	1/2,1/2,1/2	0,1,1/2	2	d	2/m	0,1/2,1/2
V	1/2,0,0	1/2,1/2,0	4	e	-1	1/4,1/4,0
L	1/2,0,1/2	1/2,1/2,1/2	4	f	-1	1/4,1/4,1/2
LD	u,u,0	0,2u,0	4	g	2	0,y,0: 0 < y < 1/2
U	u,u,1/2	0,2u,1/2	4	h	2	0,y,1/2: 0<y<1/2
B	v,-v,u	2v,0,u	4	i	m	x,0,z: 0<z<1/2; -1/2<x≤1/2 U U x,0,0: 0<x<1/2 U U x,0,1/2: 0<x<1/2
GP	u,v,w	u-v,u+v,w	8	j	1	x,y,z: 0<z<1/2; 0≤x≤1/2; 0<y<1/2 U U x,y,0: 0<x<1/4; 0<y<1/2 U U 1/4,y,0: 0<y<1/4 U U x,y,1/2: 0<x<1/4; 0<y<1/2 U U 1/4,y,1/2: 0<y<1/4

Wing: x,0,z: 0<x<1/2 -1/2<z<0

defining the parameter region (or space) of a Wyckoff position (line, plane or space) which is inside the unit cell. The ratio of order of the site-symmetry group (representing those operations which leave the parameter space *fixed pointwise*) and the order of the stabilizer (which is the set of all symmetry operations *modulo* integer translations which leave the parameter space *invariant as a whole*) gives the independent fraction of the parameter space (*i.e.* of the volume of the unit cell, or of the area of the plane, or of the length of the line). For example, the parameter space of the line $0, 0, z$ in the unit cell is determined by the variation of z in the range ($-\frac{1}{2} < z < \frac{1}{2}$). The order of the site-symmetry group is 2 while its stabilizer is of order 4 (the group $2/m$), so the independent

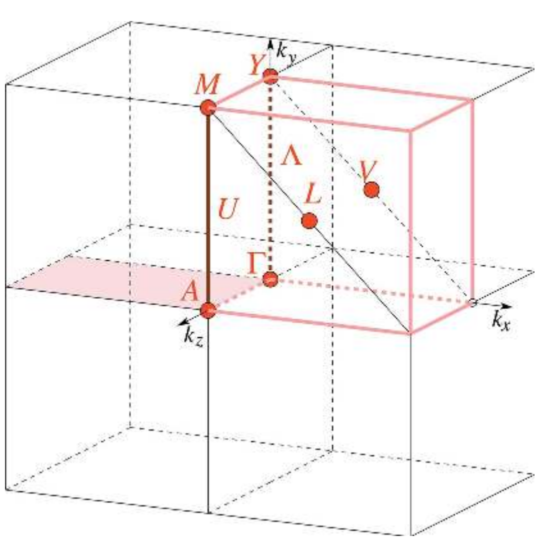

Figure 5
Unit cell and asymmetric unit of the arithmetic crystal class $12/m1C$ ($2/mC$): space groups $C12/m1$ (No. 12) and $C12/c1$ (No. 15); reciprocal-space group $(C12/m1)^*$.

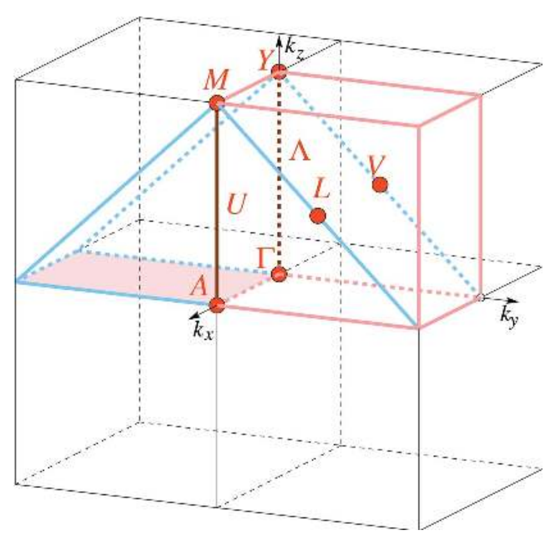

Figure 6
Unit cell, asymmetric unit and representation domain of CDML of the arithmetic crystal class $112/mA$ ($2/mC$): space groups $A112/m$ (No. 12) and $A112/a$ (No. 15); reciprocal-space group $(A112/m)^*$. The representation domain of CDML is different from the asymmetric unit.

Table 7
k-Vector tables of the space groups of the arithmetic crystal class 112/*mA* (2/*mC*) as shown on the *Bilbao Crystallographic Server*.

The unit-cell diagram is shown in Fig. 6.

The k-vector types of space group $C2/c$ (15) [unique axis c]

(Table for arithmetic crystal class 2/mC)

A112/m(C2/m) - C^3_{2h} (12), A112/a(C2/c) - C^6_{2h} (15)

Reciprocal space group (A112/m)*, No. 12

k-vector description			ITA description			
CDML		Conventional basis	Wyckoff position			Coordinates
Label	Primitive basis					
GM	0,0,0	0,0,0	2	a	2/m	0,0,0
Y	0,1/2,1/2	0,0,1	2	b	2/m	0,0,1/2
A	1/2,0,0	1/2,0,0	2	c	2/m	1/2,0,0
M	1/2,1/2,1/2	1/2,0,1	2	d	2/m	1/2,0,1/2
V	0,1/2,0	0,1/2,1/2	4	e	-1	0,1/4,1/4
L	1/2,1/2,0	1/2,1/2,1/2	4	f	-1	1/2,1/4,1/4
LD	0,u,u	0,0,2u	4	g	2	0,0,z: 0<z<1/2
U	1/2,u,u	1/2,0,2u	4	h	2	1/2,0,z: 0<z<1/2
B	u,v,-v	u,2v,0	4	i	m	x,y,0: 0<x<1/2; -1/2<y≤1/2 U U 0,y,0: 0<y<1/2 U U 1/2,y,0: 0<y<1/2
GP	u,v,w	u,v-w,v+w	8	j	1	x,y,z: 0<x<1/2; 0≤y≤1/2; 0<z<1/2 U U 0,y,z: 0<y<1/4; 0<z<1/2 U U 0,1/4,z: 0<z<1/4 U U 1/2,y,z: 0<y<1/4; 0<z<1/2 U U 1/2,1/4,z: 0<z<1/4

Wing: x,y,0: $0<x<1/2$ $-1/2<y<0$

segment is exactly $\frac{1}{2}$ of the parameter space in the unit cell, *e.g.* $(0 < z < \frac{1}{2})$. In a similar way, the independent area of the plane $x, y, 0$ is exactly $\frac{1}{2}$ of the area of the plane in the unit cell. For its uni-arm description, it is necessary to introduce a *wing*, stretching outside of the asymmetric unit $x, y, 0 : 0 < x < \frac{1}{2}, -\frac{1}{2} < y < 0$ (coloured in pink in Fig. 6).

The labels of the special **k**-vector points, lines and planes and their coordinates listed in the first two columns of Table 7 are taken directly from Table 3.9(c) of CDML. The correspondence between the special **k** vectors listed by CDML and the Wyckoff positions of ITA follows from the relation between the primitive basis $\{\mathbf{g}_1, \mathbf{g}_2, \mathbf{g}_3\}$ used by CDML and the conventional ITA basis $\{\mathbf{k}_x, \mathbf{k}_y, \mathbf{k}_z\}$ (*cf.* Table 3.4 of CDML): $\mathbf{g}_1 = \mathbf{k}_x, \mathbf{g}_2 = \mathbf{k}_y + \mathbf{k}_z, \mathbf{g}_3 = -\mathbf{k}_y + \mathbf{k}_z$ (*cf.* Fig. 6). The wave-vector coefficients (k_1, k_2, k_3) under the heading 'Conventional basis' of Table 7 refer to a basis that is dual to the conventional basis of ITA. The coefficients (k_1, k_2, k_3) are derived from the primitive coefficients (k_{p1}, k_{p2}, k_{p3}) of CDML: $k_1 = k_{p1}, k_2 = k_{p2} - k_{p3}, k_3 = k_{p2} + k_{p3}$ (*cf.* Table 2).

The **k**-vector data of $C12/c1$ (*i.e.* of the arithmetic crystal class $12/m1C$) can be derived from those of $A112/a$ (*i.e.* of $112/mA$) utilizing the relationship between the two setting descriptions of ITA. The transformation matrix **P**, specifying the relation between the basis $\{\mathbf{a}_b, \mathbf{b}_b, \mathbf{c}_b\}$ of the setting *unique axis b* (cell choice 1) and the basis $\{\mathbf{a}_c, \mathbf{b}_c, \mathbf{c}_c\}$ of the setting *unique axis c* (cell choice 1) reads

$$(\mathbf{a}_b, \mathbf{b}_b, \mathbf{c}_b) = (\mathbf{a}_c, \mathbf{b}_c, \mathbf{c}_c)\mathbf{P} = (\mathbf{a}_c, \mathbf{b}_c, \mathbf{c}_c)\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$$

(*cf.* Table 5.1.3.1 of ITA). The coordinate triplets

$$\begin{pmatrix} x_b \\ y_b \\ z_b \end{pmatrix}$$

of the special Wyckoff positions of $C12/m1$ (listed under 'ITA description' of Table 6) are obtained from the point coordinates

$$\begin{pmatrix} x_c \\ y_c \\ z_c \end{pmatrix}$$

of Table 7 by the relation

$$\begin{pmatrix} x_b \\ y_b \\ z_b \end{pmatrix} = \mathbf{P}^{-1}\begin{pmatrix} x_c \\ y_c \\ z_c \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}\begin{pmatrix} x_c \\ y_c \\ z_c \end{pmatrix} = \begin{pmatrix} y_c \\ z_c \\ x_c \end{pmatrix}.$$

For example, the representative coordinate triplet of the special Wyckoff position 4*f* of $A112/m$ transforms exactly to the representative coordinate triplet of the special Wyckoff position 4*f* of $C12/m1$:

$$\begin{pmatrix} \frac{1}{2} \\ \frac{1}{4} \\ \frac{1}{4} \end{pmatrix} \longrightarrow \begin{pmatrix} \frac{1}{4} \\ \frac{1}{4} \\ \frac{1}{2} \end{pmatrix}.$$

Under a coordinate transformation of the bases in direct space $(\mathbf{a}_b, \mathbf{b}_b, \mathbf{c}_b) = (\mathbf{a}_c, \mathbf{b}_c, \mathbf{c}_c)\mathbf{P}$, the corresponding **k**-vector coefficients transform according to $(k_{x,b}k_{y,b}k_{z,b}) = (k_{x,c}k_{y,c}k_{z,c})\mathbf{P}$ (*cf.* ITA, ch. 5.1). The transformation of the set of special **k**-vector coefficients of $A112/m$ (primitive or conventional) by the matrix

$$\mathbf{P} = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$$

results in the set of special **k**-vector coefficients for $C12/m1$ (primitive or conventional). For example, the primitive **k**-vector coefficients $(k_{p1,b}k_{p2,b}k_{p3,b})$ of $C12/m1$ are obtained from those of $A112/m$ from the relation

$$(k_{p1,b}k_{p2,b}k_{p3,b}) = (k_{p1,c}k_{p2,c}k_{p3,c}) \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$$
$$= (k_{p2,c}k_{p3,c}k_{p1,c}),$$

$$k_{p1,b} = k_{p2,c}, k_{p2,b} = k_{p3,c}, k_{p3,b} = k_{p1,c}.$$

The special **k** vectors of $C12/m1$ keep the CDML labels of the **k** vectors of $A112/m$ from which they are derived.

5. Conclusions

The wavevector database of the *Bilbao Crystallographic Server* contains Brillouin-zone figures and wavevector tables for all 230 space groups. In this compilation, the representation domains and the lists of special **k** vectors in the tables on space-group representations by Cracknell, Davies, Miller and Love (CDML) are compared with figures and wavevector data based on the so-called *reciprocal-space-group* approach which is based on the isomorphism between reciprocal-space groups and the symmorphic space groups. The database is accessed by the program *KVEC*. The **k**-vector data are the same for all space groups of the same arithmetic crystal class. There are several sets of figures and tables for the same space group when its Brillouin-zone shape depends on the lattice parameters of the reciprocal lattice. In the figures, the unit cells and asymmetric units of the symmorphic space groups chosen in ITA are juxtaposed to the Brillouin zones and representation domains of CDML. The **k**-vector data as listed by CDML are compared with the Wyckoff-position description given in ITA. The Wyckoff positions of ITA provide a complete list of the special **k** vectors of the Brillouin zones: the site-symmetry groups of ITA coincide with the little co-groups of the wavevectors; the multiplicity per primitive unit cell equals the number of arms of the **k**-vector stars. All **k**-vector stars giving rise to the same type of irreps correspond to the same Wyckoff position and applying the so-called *uni-arm description* they are collected in one entry when flagpoles and wings are admitted. Its parameter description also contains the independent parameter ranges which are essential to ensure that exactly one **k** vector per orbit is represented in the asymmetric unit or in the representation domain. In that sense, the data on the independent parameter ranges shown in the **k**-vector tables of the Brillouin-zone database provide a solution to the completeness problem of the space-group irreps.

This work has been supported by the Spanish Ministry of Science and Innovation (project MAT2012-34740) and the Government of the Basque Country (project IT779-13). EST would like to thank TUBITAK for financial support through the 2232 fellowship program. HW and MIA are grateful to L. L. Boyle who drew their attention to the article by Wintgen (1941) where the idea of the reciprocal-space-group approach was introduced for the first time.

References

Aroyo, M. I., Kirov, A., Capillas, C., Perez-Mato, J. M. & Wondratschek, H. (2006). *Acta Cryst.* A**62**, 115–128.

Aroyo, M. I., Perez-Mato, J. M., Capillas, C., Kroumova, E., Ivantchev, S., Madariaga, G., Kirov, A. & Wondratschek, H. (2006). *Z. Kristallogr.* **221**, 15–27.

Aroyo, M. I., Perez-Mato, J. M., Orobengoa, D., Tasci, E. S., de la Flor, G. & Kirov, A. (2011). *Bulg. Chem. Commun.* **43**, 183–197.

Aroyo, M. I. & Wondratschek, H. (1995). *Z. Kristallogr.* **210**, 243–254.

Boyle, L. L. (1986). *Proceedings of the 14th International Collection on Group-Theoretic Methods in Physics*, pp. 405–408. Singapore: World Scientific.

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

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

International Tables for Crystallography (2002). Vol. A, *Space-group Symmetry*, edited by Th. Hahn, 5th revised ed. Dordrecht: Kluwer Academic Publishers.

International Tables for Crystallography (2010). Vol. B, *Reciprocal Space*, edited by U. Shmueli, 3rd revised ed. Heidelberg: Springer.

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

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

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

Wintgen, G. (1941). *Math. Ann.* **118**, 195–215.