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Bilbao Crystallographic Server: I. Databases and crystallographic computing programs

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Abstract. The *Bilbao Crystallographic Server* is a web site with crystallographic databases and programs available on-line at www.cryst.ehu.es. It has been operating for about six years and new applications are being added regularly. The programs available on the server do not need a local installation and can be used free of charge. The only requirement is an Internet connection and a web browser.

The server is built on a core of databases, and contains different shells. The innermost one is formed by simple retrieval tools which serve as an interface to the databases and permit to obtain the stored symmetry information for space groups and layer groups. The **k**-vector database includes the Brillouin zones and the wave-vector types for all space groups. As a part of the server one can find also the database of incommensurate structures. The second shell contains applications which are essential for problems involving group-subgroup relations between space groups (*e.g.* subgroups and supergroups of space groups, splittings of Wyckoff positions), while the third shell contains more sophisticated programs for the computation of space-group representations and their correlations for group-subgroup related space groups. There are also programs for calculations focused on specific problems of solid-state physics. The aim of the article is to report on the current state of the server and to provide a brief description of the accessible databases and crystallographic computing programs. The use of the programs is demonstrated by illustrative examples.

1. Introduction

The *Bilbao Crystallographic Server*, URL http://www.cryst.ehu.es, is a web site with crystallographic databases and programs. It can be used free of charge from any computer with a web browser via Internet.

The server is built on a core of databases and contains different shells. The set of databases includes data from *International Tables*, Vol. A: Space-group symmetry, and the data of maximal subgroups of space groups and plane groups of index 2, 3 and 4 listed in the *International Tables* Vol. A1: Symmetry relations between Space Groups. Recently, we have started with the development of databases for the subperiodic groups: the crystallographic data for the 80 layer groups including generators, general and special positions (*International Tables* Vol. E: Subperiodic Groups) and their maximal subgroups of indices 2, 3 and 4 are already accessible on the server. Under development is a database on incommensurate structures incorporating modulated structures and composites. A **k**-vector database with Brillouin-zone figures and classification tables of the wave vectors for space groups is also available.

The communication to the databases is provided by simple retrieval tools. They form the second shell of the server and allow the access to the information on space groups or subperiodic groups in different types of formats: HTML, text ASCII or XML. In this way the retrieval tools serve not only for obtaining specific information but can also be used as input data for other programs.

The programs related to group-subgroup relations of space groups form the next shell of the server. These programs use the retrieval tools for accessing the necessary space-group information and apply group-theoretical algorithms in order to obtain specific results which are not available in the databases. Examples are the determination of different subgroups of a space group and their distribution into conjugacy classes, or the calculation of possible supergroups of a given space-group type and a fixed index. There one can find also a program for calculating the splitting rules of the Wyckoff positions for a group-subgroup pair.

It follows a shell which includes programs on representation theory of space groups and point groups and further useful symmetry information. Parallel to the crystallographic software we develop a shell with programs facilitating the study of specific problems related to solid-state physics, structural chemistry and crystallography.

The server has been operating for almost six years, and new programs and applications are being added (Kroumo-

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va *et al.* 1998b, 1999, 2003). The aim of the present contribution is to report on the current state of the server and to provide a description of the different databases and the retrieval tools which allow the access of the stored symmetry information (Section 2). The discussion of the accompanying applications is focused on the crystallographic computing programs which form the second shell of the server (Section 3). Here the underlying group-theoretical background of the developed programs is briefly explained and more details on the necessary input data and the outcoming results are given. The use of the programs is demonstrated by illustrative examples. The rest of the available programs is the subject of a forthcoming article.

2. Databases and retrieval tools

The databases form the core of the *Bilbao Crystallographic Server*. The information contained in these databases is used by all of the programs available on the server.

2.1. Space-group data

The space-group databases include the following symmetry information:

- The data on the 230 space groups as listed in the *International Tables for Crystallography*, Vol. A (1995, hereafter referred to as *IT*A) including generators and general positions, Wyckoff positions and Wyckoff sets, affine and Euclidean normalizers, types of maximal subgroups, and types of minimal supergroups. The data from the databases can be accessed using the simple retrieval tools GENPOS, WYCKPOS, NORMALIZER and WYCKSETS. All of them use as input the number of the space group as given in the *IT*A (*IT*A-numbers), but there is always a possibility to select the group from a table with *IT*A-numbers and Hermann-Mauguin symbols. The output of GENPOS contains the list with the generators or the general positions and provides the possibility to obtain the same data in different settings either by specifying the transformation matrix to the new basis or selecting one of the 530 settings listed in Table 4.3.2.1 of *IT*A. The list with the Wyckoff positions for a given space group in different settings can be obtained using the program WYCKPOS. The program NORMALIZER is used to access the data on affine and Euclidean normalizers of the space groups. They are described by sets of additional symmetry operations that generate the normalizers successively from the space groups (*cf.* *IT*A, Table 15.2). In the case of triclinic and monoclinic groups only the Euclidean normalizers corresponding to general metric conditions are available for the moment. The assignments of the Wyckoff positions to Wyckoff sets (*cf.* Koch and Fischer, 1975) are retrieved by the program WYCKSETS. In addition, the output gives a list of the coset representatives of the decompositions of the normalizers with respect to the space groups and the transformation of the Wyckoff positions under the action of these coset representatives.
- The list with the maximal subgroups $\mathcal{H}$ of indices 2, 3 and 4 of the space groups $\mathcal{G}$. This information forms part of the Volume A1 of the *International Tables for Crystallography* (2004, referred to as *IT*A1). There, each subgroup is listed individually and is specified either by a set of general-position representatives or by a set of generators. All maximal non-isomorphic subgroups and maximal isomorphic subgroups of index 2, 3 and 4 of each space group can be retrieved from the database using the program MAXSUB. Each subgroup $\mathcal{H}$ is specified by its *IT*A-number, the index in the group $\mathcal{G}$ and the transformation matrix-column pair ($\boldsymbol{P}$, $\boldsymbol{p}$). The 3×3 square matrix $\boldsymbol{P} = \|P_{ij}\|$ transforms the conventional basis $(\mathbf{a}, \mathbf{b}, \mathbf{c})_{\mathcal{G}}$ of $\mathcal{G}$ to the conventional basis of $\mathcal{H}$:

$$(\mathbf{a}', \mathbf{b}', \mathbf{c}')_{\mathcal{H}} = (\mathbf{a}, \mathbf{b}, \mathbf{c})_{\mathcal{G}}\, \boldsymbol{P}\,. \qquad (1)$$

  The column $\boldsymbol{p} = (p_1, p_2, p_3)$ of coordinates of the origin $O_{\mathcal{H}}$ of $\mathcal{H}$ is referred to the coordinate system of $\mathcal{G}$. Hereafter, the data on the matrix-column pair ($\boldsymbol{P}$, $\boldsymbol{p}$) are often written in the following concise form:

$$\begin{array}{ll} P_{11}\mathbf{a} + P_{21}\mathbf{b} + P_{31}\mathbf{c}\,, & P_{12}\mathbf{a} + P_{22}\mathbf{b} + P_{32}\mathbf{c}\,, \\ P_{13}\mathbf{a} + P_{23}\mathbf{b} + P_{33}\mathbf{c}\,; & p_1, p_2, p_3\,. \end{array} \qquad (2)$$

  For certain applications it is necessary to represent the subgroups $\mathcal{H}$ as subsets of the elements of $\mathcal{G}$. This is achieved by an option in MAXSUB which transforms the general-position representatives of $\mathcal{H}$ by the corresponding matrix-column pair ($\boldsymbol{P}$, $\boldsymbol{p}$) to the coordinate system of $\mathcal{G}$.
  Here, as well as in all programs related to maximal subgroups (or minimal supergroups), the following *IT*A conventional settings are chosen as standard (hereafter also referred to as default settings): *unique axis b* setting for monoclinic groups, *hexagonal axes* setting for rhombohedral groups, and *origin choice 2* for the centrosymmetric groups listed with respect to two origins in *IT*A.

Most of space-group data are stored in a provisional CIF format. For the extension of the existing CIF-core dictionary, a list of data names has been compiled for the space groups and their subgroups (Wondratschek, Madariaga and Aroyo, 1996).

2.2 Subperiodic groups

Recently, we have started with the development of a database for the subperiodic groups with symmetry information as listed in *International Tables* Vol. E: Subperiodic Groups (hereafter referred to as *IT*E). For the moment the Bilbao Crystallographic Server provides a free on-line access to a database for the 80 layer groups including generators, general and special positions. The structure of this database and the retrieval programs are similar to the *IT*A database.

In addition, the complete information on maximal subgroups of layer groups (Aroyo Wondratschek, 2004) is made available: Similar to the *IT*A1 database, all maximal

non-isotypic subgroups as well as maximal isotypic subgroups of index 2, 3 and 4 are listed individually. The conjugacy relations of the subgroups in the original group are indicated. The transformation to the conventional coordinate system of the subgroup is available as a 3×3 matrix for the change of basis and a column for the origin shift. Each subgroup can be further specified by its general-position representatives referred to the basis of the group. The symmetry information has been stored in a provisional CIF-format. For the extension of the existing CIF-core dictionary a list of data names has been developed which refer to the specific requirements of the subgroup tables of the layer groups.

2.3 k-vectors and Brillouin zones

The determination, classification, labeling and tabulation of irreducible representations (irreps) of space groups is based on the use of wave vectors **k**. The **k**-vector database available on the Bilbao Crystallographic Server contains figures of the Brillouin zones and tables which form the background of a classification of the irreps of all 230 space groups. In this compilation the symmetry properties of the wave vectors are described by the so-called reciprocal-space groups which are isomorphic to symmorphic space groups (Wintgen, 1941, see also Aroyo Wondratschek, 1995). This isomorphism allows the application of crystallographic conventions in the classification of the wave vectors (and henceforth in the irreps of the space groups). For example, the different symmetry types of **k**-vectors correspond to the different kinds of point orbits (Wyckoff positions) in the symmorphic space groups; the unit cells with the asymmetric units given in *IT*A can serve as Brillouin zones and representation domains, *etc.* The advantages of the reciprocal-space group approach compared to the traditional schemes of wave-vector classification can be summarized as follows:

- The asymmetric units given in *IT*A serve as representation domains which are independent of the different shapes of the Brillouin zones for different ratios of the lattice parameters.
- For the non-holohedral groups the representation domain is obtained from that of the corresponding holohedral group by extending the parameter ranges, not by introducing differently labeled special **k**-vector points, lines or planes of symmetry.
- A complete list of the special sites in the Brillouin zone is provided by the Wyckoff positions of *IT*A. The site symmetry of *IT*A corresponds to the little co-group of the wave vector; the number of branches of the star of **k** follows from the multiplicity of the Wyckoff position.
- All **k**-vector stars giving rise to the same type of irreps are related to the same Wyckoff position and designated by the same Wyckoff letter.

The available figures and the wave-vector data based on the reciprocal-space group symmetry are compared with the representation domains and the **k**-vector tables of the widespread tables of space-group representations by Cracknell, Davies, Miller and Love (1979, hereafter referred to as CDML).

The retrieval tools of the **k**-vector database use as input the *IT*A-number of the space group. The output contains wave-vector 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 tables, the **k**-vector data as listed by CDML are compared with the Wyckoff-position description as given in *IT*A. Each **k**-vector type is specified by its label and parameters. The corresponding Wyckoff positions are described by their Wyckoff letters, multiplicities, and site symmetry groups. Their parameter description contains also the parameter ranges chosen in such a way that each orbit of the Wyckoff position of *IT*A, *i.e.* also each **k**-orbit, is listed *exactly once*. No ranges for the parameters are listed in CDML. Symmetry points, lines of symmetry or planes of CDML which are related to the same Wyckoff position are grouped together.

In the figures, the Brillouin zones of CDML and the conventional unit cells of *IT*A 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 *IT*A. The names of **k**-vector points, lines, and planes of CDML are retained in this listing. New names have been given only to points and lines which are not listed in CDML.

2.3.1 Example

The following example illustrates the relation between the traditional and the reciprocal-space group descriptions of the wave-vector types of space-group irreps.

Arithmetic crystal class $222F$. This arithmetic crystal class consists accidentally of only one space group:

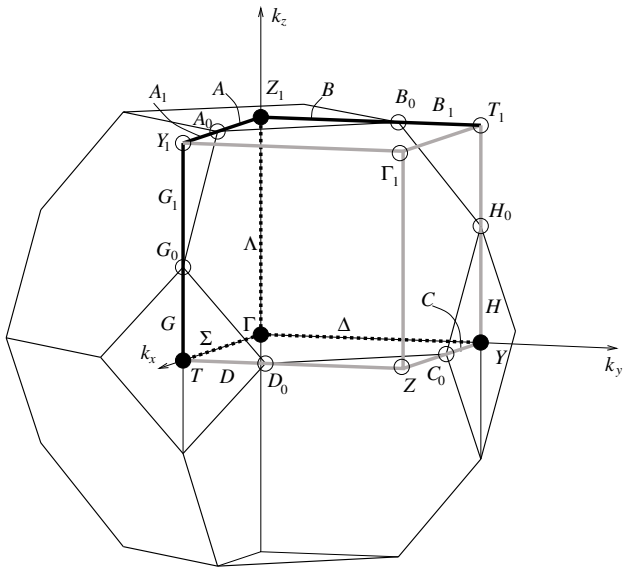

Fig. 1. Brillouin zone for the arithmetic crystal class $222F$: $a^{-2} < b^{-2} + c^{-2}$, $b^{-2} < c^{-2} + a^{-2}$ and $c^{-2} < a^{-2} + b^{-2}$. The representation domain (RD) is given by the vertices A_0, B_0, Z_1, G_0, H_0, D_0, C_0 and the corresponding vertices with the negative k_z coordinates. The asymmetric unit (AU) is the rectangular prism with the vertices Γ, T, Z, Y, Z_1, Y_1, Γ_1 and T_1. Black vertices are special points of the RD (and AU); black (thick) and grey (thick) lines are edges of the AU.

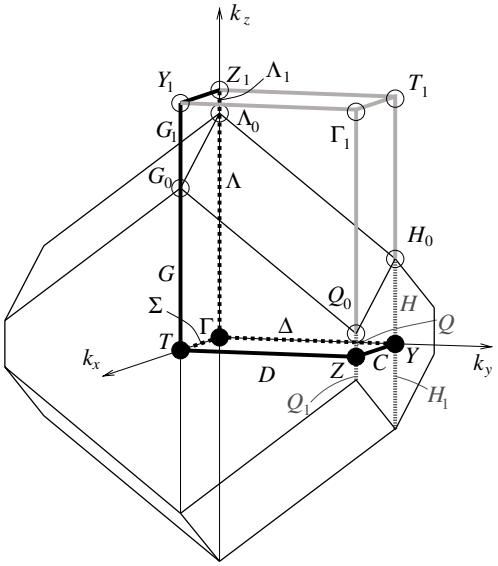

Fig. 2. Brillouin zone for the arithmetic crystal class $222F$: $c^{-2} > a^{-2} + b^{-2}$. The representation domain (RD) is the body with the vertices Λ_0, G_0, Q_0, H_0 and the corresponding vertices with the negative k_z coordinates. The asymmetric unit (AU) is the rectangular prism with the vertices Γ, T, Z, Y, Z_1, Y_1, Γ_1 and T_1. Black vertices are special points of the RD (and AU); black (thick) and grey (thick) lines are edges of the AU; the grey (dashed) lines H_1 and Q_1 are special lines of the RD which are represented in the AU by the lines G_1 and Λ_1.

$F222 \sim D_2^7$, the reciprocal space group is isomorphic to $I222 \sim D_2^8$. Depending on the relations between the lattice constants a, b and c, there are two topologically different bodies of the Brillouin zone displayed in Fig. 1 and Fig. 2 by thin black lines; the first one has 24 vertices, 36 edges and 14 faces, the other has 18 vertices, 28 edges and 12 faces. The shape of the unit cell of *IT*A is always a parallelepipedon with 8 vertices, 12 edges and 6 faces. Similarly, the representation domains (abbreviated RD) of CDML are more complicated than the asymmetric units (abbreviated AU) of *IT*A, see Fig. 1 and Fig. 2.

To save space we have included only part of the table of **k**-vector relations for the arithmetic crystal class $222F$ in Table 1, corresponding to Fig. 1. The **k**-vector parameters of CDML (second column) of Table 1 are different from those of *IT*A (last column) because in CDML the data are always referred to a primitive basis, whereas in *IT*A they are referred to a centered basis if appropriate, *e.g.* in F and I lattices. The parameter ranges (last column) are chosen such that each **k**-vector orbit is represented exactly once.

One takes from Table 1 that different **k** labels of CDML (first column) may belong to the same type of **k** vectors, *i.e.* they give rise to the same type of irreps. Due to the special shape of the representation domain of CDML the special wave-vector line corresponding to the Wyckoff position $4f$ (2..) (third column) is split into two parts, A and C. In the *IT*A description $A \cup C$ corresponds to one line $[Z_1Y_1]$, $(x, 0, {}^1/_2)$, with $0 < x < {}^1/_2$. The splitting of the $4f$ line into two parts is a consequence of the Brillouin-zone shape for the specific values of the lattice parameters. This is confirmed from Fig. 2 where the corresponding special line C is not split.

2.4 Incommensurate Crystal Structure Database

As a part of the *Bilbao Crystallographic Server* one can also find a database of incommensurate structures (ICSDB). The necessity of such a database is justified by the specific description of these structures due to which they cannot be included in the 'conventional' crystal-structure databases. ICSDB contains both single modulated structures and composites. ICSDB is different from the rest of the server databases in the sense that it is designed so that the user cannot only access the data, but also has the possibility to add new structures (on-line input).

The tools available for the access to the database permit the search for a given structure specified by the author(s) and/or chemical element(s). The result from a specific search contains the list with the compounds that satisfy the search conditions and a link to the full information for each structure. Also, there is a possibility to obtain the CIF file with the structure data.

New structures can be added either by using a specially designed web-interface, or the data can be sent via e-mail using the CIF format. Each structure is provided with a unique ID and password which permits the author to edit the data.

The structures resolved with the program JANA (Petříček & Dušek, 1998) can be added to the database directly, using the output of the program. It is only necessary to provide some additional information as author(s) name(s), the publication data, and the e-mail address for contact.
ICSDB is accessible at: http://www.cryst.ehu.es/icsdb/

k-vector label CDML			Wyckoff position *IT*A			Parameters, see Fig.1 *IT*A
Γ	0, 0, 0		2	a	222	0, 0, 0
T	0, ${}^1/_2$, ${}^1/_2$		2	b	222	${}^1/_2$, 0, 0
$Z_1 (\sim Z)$	${}^1/_2$, ${}^1/_2$, 0		2	c	222	0, 0, ${}^1/_2$
Y	${}^1/_2$, 0, ${}^1/_2$		2	d	222	0, ${}^1/_2$, 0
Σ	$0, \alpha, \alpha$		4	e	2..	x, 0, 0: $0 < x < {}^1/_2$
A	${}^1/_2$, ${}^1/_2 + \alpha$, α	ex	4	f	2..	x, 0, ${}^1/_2$: $0 < x \leq a_0$
C	${}^1/_2$, α, ${}^1/_2 + \alpha$	ex	4	f	2..	x, ${}^1/_2$, 0: $0 < x < c_0$
$C \sim A_1 = [A_0Y_1]$						x, 0, ${}^1/_2$: $a_0 < x < {}^1/_2$
$A \cup A_1 = [Z_1Y_1]$			4	f	2..	x, 0, ${}^1/_2$: $0 < x < {}^1/_2$

Table 1. Selection of the **k**-vector types for the arithmetic crystal class $222F$ (Space group $F222 - D_2^7(22)$): $a^{-2} < b^{-2} + c^{-2}$, $b^{-2} < c^{-2} + a^{-2}$ and $c^{-2} < a^{-2} + b^{-2}$. The **k**-vector labels and parameters of CDML are compared with the Wyckoff positions of *IT*A for the symmorphic space group $I222$, isomorphic to the reciprocal-space group of $222F$. 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 $x = {}^1/_2(-k_1 + k_2 + k_3)$, $y = {}^1/_2(k_1 - k_2 + k_3)$, $z = {}^1/_2(k_1 + k_2 - k_3)$.

3. Crystallographic computing programs

The data from the databases, obtained using the retrieval tools described above, are used in more sophisticated algorithms to obtain information which is not directly accessible from the databases and which is necessary for the solution of different crystallographic problems. These programs form the second shell of the *Bilbao Crystallographic Server.*

3.1 Subgroups of space groups

The problem

If two space groups $\mathcal{G}$ and $\mathcal{H}$ form a group-subgroup pair $\mathcal{G} > \mathcal{H}$, it is always possible to represent their relation by a chain of intermediate maximal subgroups $\mathcal{Z}_k$: $\mathcal{G} > \mathcal{Z}_1 > \ldots > \mathcal{Z}_n = \mathcal{H}$. For a specified index of $\mathcal{H}$ in $\mathcal{G}$ there are, in general, a number of possible chains relating both groups, and a number of different subgroups $\mathcal{H}_j < \mathcal{G}$ isomorphic to $\mathcal{H}$.

The program SUBGROUPGRAPH (Ivantchev *et al.*, 2000), analyzes the group-subgroup relations between space groups. Its results can be summarized as follows:

- Given the space groups $\mathcal{G}$ and $\mathcal{H}$ with unspecified index, the program determines the $\mathcal{G} - \mathcal{H}$ lattice of maximal subgroups containing the space-group types of all possible intermediate groups $\mathcal{Z}_k$.
- If the index of $\mathcal{H}$ in $\mathcal{G}$ is specified, the program determines all possible chains of maximal subgroups relating $\mathcal{G}$ and $\mathcal{H}$, the different subgroups $\mathcal{H}_j$ of $\mathcal{G}$ with the given index, and their distribution into classes of conjugate subgroups with respect to $\mathcal{G}$.

In addition, the group-subgroup lattice and the chains of maximal subgroups relating $\mathcal{G}$ and $\mathcal{H}$ are represented as graphs with vertices corresponding to the space groups involved.

The method

The program is based on the data for the maximal subgroups of index 2, 3 and 4 of the space groups of *IT*A1. These data are transformed into a graph with 230 vertices corresponding to the 230 space-group types. If two vertices in the graph are connected by an edge, the corresponding space groups form a group − maximal-subgroup pair. Each one of these pairs is characterized by a group-subgroup index. The different maximal subgroups of the same space-group type are distinguished by corresponding matrix-column pairs ($\boldsymbol{P}$, $\boldsymbol{p}$) which give the relations between the conventional coordinate systems of the group and the subgroup. The index and the set of transformation matrices are considered as attributes of the edge connecting the group with the subgroup.

The specification of the group − subgroup pair $\mathcal{G} > \mathcal{H}$ leads to a reduction of the total graph to a subgraph with $\mathcal{G}$ as the top vertex and $\mathcal{H}$ as the bottom vertex. In addition, the $\mathcal{G} > \mathcal{H}$ subgraph, referred to as the *general* $\mathcal{G} > \mathcal{H}$ graph, contains all possible groups $\mathcal{Z}_k$ which appear as intermediate maximal subgroups between $\mathcal{G}$ and $\mathcal{H}$. It is important to note that in the general $\mathcal{G} > \mathcal{H}$ graphs the space-group symbols indicate space-group types, *i.e.* all space groups belonging to the same space-group type are represented by one node on the graph. Such graphs are called *contracted.* The contracted graphs should be distinguished from the *complete* graphs where all space groups occurring in group-subgroup graphs are indicated by different space-group nodes.

The number of the vertices in the general $\mathcal{G} > \mathcal{H}$ graph may be further reduced if the index of $\mathcal{H}$ in $\mathcal{G}$ is specified. The obtained subgraph is again of contracted type.

Different chains of maximal subgroups for the group-subgroup pair $\mathcal{G} > \mathcal{H}$ are obtained following the possible paths connecting the top of the graph (the group $\mathcal{G}$) with the bottom (the group $\mathcal{H}$). Each group − maximal subgroup pair determines one step of this chain. The index of $\mathcal{H}$ in $\mathcal{G}$ equals the product of the indices for each one of the intermediate edges. The transformation matrices, relating the conventional bases of $\mathcal{G}$ and $\mathcal{H}$, are obtained by multiplying the matrices of each step of the chain. Thus, for each pair of group-subgroup types with a given index, there is a set of transformation matrices $(\boldsymbol{P}, \boldsymbol{p})_j$, where each matrix corresponds to a subgroup $\mathcal{H}_j$ isomorphic to $\mathcal{H}$. Some of these subgroups could coincide. To find the different $\mathcal{H}_j$ of $\mathcal{G}$, the program transforms the elements of the subgroup $\mathcal{H}$ in the basis of the group $\mathcal{G}$ using the different matrices $(\boldsymbol{P}, \boldsymbol{p})_j$, and compares the elements of the subgroups $\mathcal{H}_j$ in the group basis. Two subgroups that are characterized by different transformation matrices are considered identical if their elements, transformed to the basis of the group $\mathcal{G}$, coincide.

The different subgroups $\mathcal{H}_j$ are further distributed into classes of conjugate subgroups with respect to $\mathcal{G}$ by checking directly their conjugation relations with elements of $\mathcal{G}$.

3.1.1 The program SUBGROUPGRAPH

Input information

- As an input the program needs the specification of the space groups $\mathcal{G}$ and $\mathcal{H}$. The groups $\mathcal{G}$ and $\mathcal{H}$ can be defined either by their sequential *IT*A numbers or by their Hermann-Mauguin symbols. The default settings are used for the monoclinic and the rhombohedral space groups as well as for the centrosymmetrical groups listed with respect to two origins in *IT*A.
- If the index of $\mathcal{H}$ in $\mathcal{G}$ is specified, then the program determines the chains of maximal subgroups relating these groups and classifies the isomorphic subgroups $\mathcal{H}_j$ into classes of conjugate subgroups. If the index is not specified, then the result is the lattice of all maximal subgroups $\mathcal{Z}_k$ that relate $\mathcal{G}$ and $\mathcal{H}$.

Output information

1. Lattice of maximal subgroups relating $\mathcal{G}$ and $\mathcal{H}$ with non-specified index.
   When the index of the subgroup $\mathcal{H}$ in $\mathcal{G}$ is not specified, the program returns as a result the list of the possible intermediate space groups $\mathcal{Z}_k$ relating $\mathcal{G}$ and $\mathcal{H}$. The list is given in the form of a table whose rows correspond to the intermediate space groups $\mathcal{Z}_k$, specified by their Hermann-Mauguin symbols. In addition, the table contains the maximal

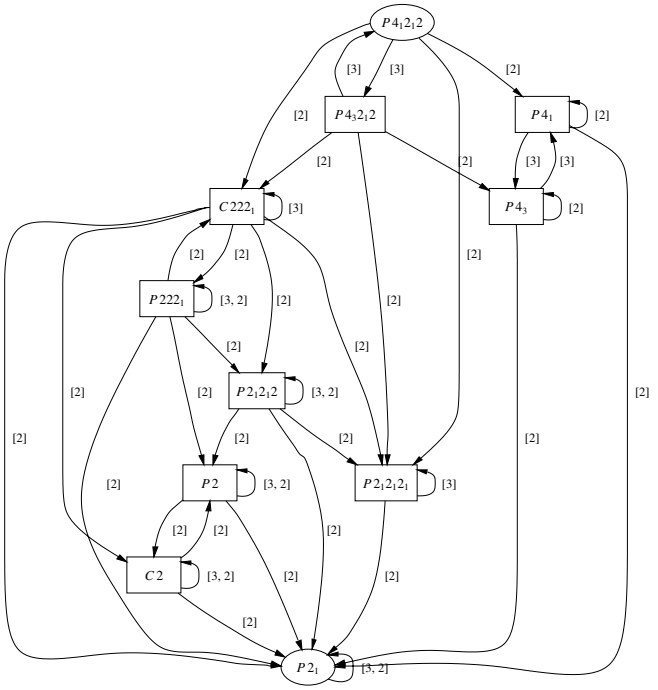

Fig. 3. General contracted graph for $P4_12_12 > P2_1$. The nodes of the graph correspond to the types of space groups that can appear as intermediate subgroups in the chains of the group-subgroup pair $P4_12_12 > P2_1$. Each edge of the graph corresponds to a group-maximal subgroup pair of the indicated index $[i]$. The loops correspond to isomorphic subgroups.

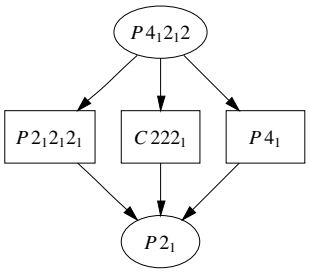

Fig. 4. Contracted graph for the pair of space groups $P4_12_12 > P2_1$, index 4. The nodes correspond to space-group types. The directed edges represent the possible group-maximal subgroup pairs.

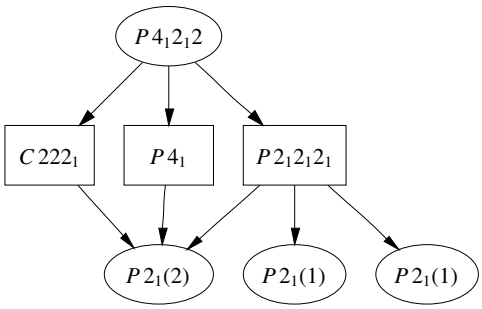

Fig. 5. Complete graph for $P4_12_12 > P2_1$, index 4. The nodes represent space groups and not space-groups types. The three subgroups of the type $P2_1$ are distributed into two classes of conjugate subgroups which are indicated in the parentheses after the space-group symbol. The two subgroups $P2_1(1)$ belonging to the same conjugacy class have identical single graphs, which considerably differ from the graph of $P2_1(2)$.

subgroups of $\mathcal{Z}_k$, specified by their *IT*A-numbers and the corresponding indices given in brackets.
This list is represented also as a contracted graph. Each space group in the list corresponds to one vertex in the graph, and its maximal subgroups are the neighbors (successors) of this vertex. Group-subgroup relations in both directions are represented by vertices connected with two lines. Maximal isomorphic subgroups are shown by loop edges (vertices connected to themselves), *cf.* Fig. 3.

2. Chains of maximal subgroups relating $\mathcal{G}$ and $\mathcal{H}$ with a given index. As an example, *cf.* Table 2 and Figs. 4 and 5.
If the index of the subgroup $\mathcal{H}$ in the group $\mathcal{G}$ is specified, the program returns a list with all of the possible chains of maximal subgroups relating $\mathcal{G}$ and $\mathcal{H}$ with this index. (Please note, that for the moment the program has no access to the data on maximal isomorphic subgroups with indices higher than four.) The number of different transformation matrices as well as a link to the list with these matrices are given for each of the possible chains.
The graphical representation contains the intermediate groups that connect $\mathcal{G}$ and $\mathcal{H}$ with the specified index. This graph is a subgraph of the general graph of maximal subgroups with unspecified index and is also of contracted type.
3. Classification of the different subgroups $\mathcal{H}_j$ of $\mathcal{G}$.
Once the index of $\mathcal{H}$ in $\mathcal{G}$ is given, and the chains relating these groups with the corresponding index are obtained, the different subgroups are calculated and distributed into classes of conjugate subgroups. The distribution of the subgroups $\mathcal{H}_j$ into classes of conjugate subgroups can be compared with the corresponding results obtained by the application of the normalizer procedure described by Koch (1984).
Each class of conjugate subgroups is represented in a table which contains the chains and the transformation matrices used to obtain the subgroups in this class. There is also a link to a list of the elements of the subgroups transformed to the basis of the group.
The graph in this case contains the same space-group types $\mathcal{Z}_k$ as the graph of the previous step but the different isomorphic subgroups are represented by different vertices, *i.e.* the graph is a complete one. At the bottom of the graph are given all isomorphic subgroups $\mathcal{H}_j$. Their labels are formed by

Table 2. Group-subgroup relations for $P4_12_12 > P2_1$, index 4. There are three different subgroups $\mathcal{H}_j = (P2_1)_j$ of $P4_12_12$ distributed into 2 classes of conjugate subgroups. The possible chains of maximal subgroups and the corresponding matrices $(\boldsymbol{P}, \boldsymbol{p})_k$ (written in concise form) are also shown.

	$\mathcal{H}_j$	Chains	$(\boldsymbol{P}, \boldsymbol{p})_j$
Class 1	$(P2_1)_1$	$P4_12_12 > P2_12_12_1 > P2_1$	$\mathbf{a}, \mathbf{b}, \mathbf{c}$; $1/4\ 0\ 5/8$
	$(P2_1)_2$	$P4_12_12 > P2_12_12_1 > P2_1$	$\mathbf{c}, \mathbf{a}, \mathbf{b}$; $1/4\ 1/4\ 3/8$
Class 2	$(P2_1)_3$	$P4_12_12 > P2_12_12_1 > P2_1$	$\mathbf{b}, \mathbf{c}, \mathbf{a}$; $1/2\ 0\ 3/8$
		$P4_12_12 > P4_1 > P2_1$	$\mathbf{b}, \mathbf{c}, \mathbf{a}$; $0\ 1/2\ 0$
		$P4_12_12 > C222_1 > P2_1$	$\mathbf{a}, \mathbf{c}, -\mathbf{b}$; $0\ 0\ 1/4$

the symbol of the subgroup followed by a number given in parenthesis which specifies the class of conjugate subgroups to which the subgroup $\mathcal{H}_j$ belongs.

Note that for group-subgroup pairs with high indices, where a lot of intermediate maximal subgroups occur, the resulting complete graph with all subgroups $\mathcal{H}_j$ could be very complicated and difficult to overview. Alternatively, a more simple graph associated to a single specific subgroup $\mathcal{H}_j$ (equal for all subgroups within a conjugacy class) can also be obtained.

URL of the program

http://www.cryst.ehu.es/cryst/subgroupgraph.html

Example

As an example we consider the group-subgroup relations between the groups $\mathcal{H} = P2_1$ (*IT*A No. 4) and $\mathcal{G} = P4_12_12$ (*IT*A No. 92). If no index is specified then the lattice of maximal subgroups that relate $P4_12_12$ and $P2_1$ is represented as a table indicating the space-group types of the possible intermediate space groups $\mathcal{Z}_k$, and the corresponding indices. The contracted general $P4_12_12 > P2_1$ graph is shown in Fig. 3. The double directed edges between the groups correspond to group-subgroup relations in both directions, *e.g.*, the pair $P4_1$ and $P4_3$. When the index $[i]$ of the subgroup in the group is specified, the resultant graph is reduced to the chains of maximal subgroups that correspond to the value of $[i]$. For example, in Fig. 4 the contracted graph $P4_12_12 > P2_1$ of index 4 is shown. Based on the *IT*A1 data the program has found 5 possible chains $P4_12_12 > P2_1$ each specified by different transformations $(\boldsymbol{P}, \boldsymbol{p})_j$, with $j = 1, \ldots, 5$. However, further analysis of the group-subgroup relations (option 'Classify subgroups') shows that there are only 3 different $P2_1$ subgroups of $P4_12_12 > P2_1$ of index 4, distributed in two classes of conjugate subgroups (Table 2). The complete $P4_12_12 > P2_1$ graph on Fig. 5 shows that three different maximal subgroup chains end to the same $P2_1$ subgroup. The three different subgroups of space-group type $P2_1$ obviously correspond to the three two-fold screw axes in $P4_12_12$: those, pointing along the x and y axes, give rise to the two conjugated subgroups, and the third one (forming a class of conjugate subgroups by itself) is along the tetragonal axis. The corresponding transformations are listed in the Table 2.

The comparison between the complete graph (Fig. 5) and the contracted one (Fig. 4) shows that the use of contracted graphs for the analysis of specific group-subgroup relations $\mathcal{G} > \mathcal{H}_j$ can be very misleading. Obviously, subgroups $\mathcal{H}_j$ belonging to the same conjugacy class with respect to $\mathcal{G}$ have topologically the same complete graphs.

3.1.2 The program CELLSUB

The program CELLSUB has been designed as a complementary tool of the SUBGROUPGRAPH module. According to a theorem of Hermann (Hermann, 1929) for each pair $\mathcal{G} > \mathcal{H}$, there exists a uniquely defined intermediate subgroup $\mathcal{M}$, $\mathcal{G} \geq \mathcal{M} \geq \mathcal{H}$, such that $\mathcal{M}$ is a *translationengleiche* or *t*-subgroup in $\mathcal{G}$, and $\mathcal{H}$ is a *klassengleiche*, or *k*-subgroup in $\mathcal{M}$. Hence, the index $[i]$ of $\mathcal{H}$ in $\mathcal{G}$, can be decomposed in two factors $[i] = [i_t] \cdot [i_k]$. The first one is the so-called *t*-index $[i_t]$, which is related to the reduction of the point-group symmetry operations in the subgroup. The second one is known as the *k*-index $[i_k]$, and it takes account of the loss of translations. (The *k*-index is equal to the cell-multiplication factor of the primitive cells.) The program CELLSUB calculates the different subgroups of a space group $\mathcal{G}$ for a given maximum *k*-index $[i_k]$ in two steps:

- Determines all possible space-group types $\mathcal{H}^m$ which form group-subgroup pairs with $\mathcal{G}$, $\mathcal{G} > \mathcal{H}^m$ of index $[i] = [i_t] \cdot [i_k]$, such that the *k*-factor $[i_k]$ is smaller than a given value $[(i_k)_{\max}]$.
- For each pair of space-group types $\mathcal{G} > \mathcal{H}^m$ and their index $[i]$ satisfying the above condition, CELLSUB finds all possible subgroups $\mathcal{H}_j^m$, specified by the matrix-column pairs $(\boldsymbol{P}, \boldsymbol{p})_j^m$ and classifies them into classes of conjugate subgroups.

The method for obtaining the different subgroup types and indices of a given space group $\mathcal{G}$ is somehow similar to that used in the SUBGROUPGRAPH module and it is also based on the data on maximal subgroups of the space groups of *IT*A1.

Input information

- The space group $\mathcal{G}$: The space group can be specified either by its sequential *IT*A number, or by its Hermann-Mauguin symbol. Note that the program uses the default settings for the monoclinic, rhombohedral and centrosymmetrical groups listed with two origins in *IT*A.
- The (maximum) *k*-index. By default (full-list option), all subgroups with a *k*-index smaller than the given $[(i_k)_{\max}]$ are shown. As an option, it is possible to choose only the subgroups with the specified (maximum) *k*-index.

Output information

- The list of the space-group types of the subgroups $\mathcal{H}^m$ with the corresponding index $[i]$, the *t*-index $[i_t]$ and the *k*-index $[i_k]$, $[i_k] = [i]/[i_t]$. The subgroups are further classified into *k*-subgroups, *t*-subgroups (for the special case of $[i_k] = 1$) or general subgroups.
- The link to the SUBGROUPGRAPH module provides for every space-group type $\mathcal{H}^m$ of the list: the chains of maximal subgroups relating $\mathcal{G}$ and $\mathcal{H}^m$ with the given index, the classification of the different subgroups $\mathcal{H}_j^m$ of $\mathcal{G}$ in classes of conjugate subgroups, the graphical representations and all the benefits of the program SUBGROUPGRAPH.

URL of the program

http://www.cryst.ehu.es/cryst/cellsub.html

3.2 Supergroups of space groups

The problem

The problem of the determination of the supergroups of a given space group is of rather general interest. For different applications it is not sufficient to know only the space-

group types of the supergroups of a given group; it is rather necessary to have available all different supergroups $\mathcal{G}_k > \mathcal{H}$ which are isomorphic to $\mathcal{G}$, and are of the same index $[i]$. In the literature, there are very few papers treating the supergroups of space groups in any detail (Koch, 1984; Wondratschek and Aroyo, 2001). In *IT*A one finds only listings of minimal supergroups of space groups which, in addition, are not explicit: they only provide for each space group $\mathcal{H}$ the list of those space-group types in which $\mathcal{H}$ occurs as a maximal subgroup. It is not trivial to determine all supergroups $\mathcal{G}_k > \mathcal{H}$ if only the types of the minimal supergroups are known. The program SUPERGROUPS (Ivantchev *et al.*, 2002) solves this problem for a given finite index $[i]$.

The method

Let $\mathcal{G}$ be a space group and $\mathcal{H} < \mathcal{G}$ one of its maximal subgroups of index $[i]$. Then all subgroups $\mathcal{H}_j$ which are maximal subgroups of $\mathcal{G}$ of the same index $[i]$ and are isomorphic to $\mathcal{H}$ are listed in *IT*A1. The number of maximal subgroups with index $[i]$ is finite for any space group. Therefore, such a list is always finite.

Let $\mathcal{H} < \mathcal{G}$ be a member of this list for the space group $\mathcal{G}$ and index $[i]$. Then one wants to know for the space group $\mathcal{H}$ all minimal supergroups $\mathcal{G}_k > \mathcal{H}$ of index $[i]$ which are isomorphic to $\mathcal{G}$, $\mathcal{G}_k \cong \mathcal{G}$. According to the Theorem of Bieberbach, for space groups isomorphism and affine equivalence result in the same classification. Therefore, one is looking for the set of all minimal supergroups $\mathcal{G}_k$ of $\mathcal{H}$ of index $[i]$ which are affinely equivalent to $\mathcal{G}$, $\mathcal{G}_k \sim \mathcal{G}$. Then there must be a mapping $a_k \in \mathcal{A}$ such that $a_k^{-1}\mathcal{G}\,a_k = \mathcal{G}_k$, where A is the group of all reversible affine mappings.

There are two cases to be distinguished.

1. The first candidates for the mapping a_k are the elements of the affine normalizer of $\mathcal{H}$, *i.e.* $a_k \in \mathcal{N}_{\mathcal{A}}(\mathcal{H})$. If $a_k \in \mathcal{N}_{\mathcal{A}}(\mathcal{H})$, $\mathcal{H}$ is mapped onto itself by the transformation with a_k and $\mathcal{G}_k = a_k^{-1}\mathcal{G}a_k$ is a minimal supergroup of $\mathcal{H}$. More exactly, because of $\mathcal{N}_{\mathcal{A}}(\mathcal{H}) \geq (\mathcal{N}_{\mathcal{A}}(\mathcal{H}) \cap \mathcal{N}_{\mathcal{A}}(\mathcal{G})) = \mathcal{D} \geq \mathcal{H}$, the transformation with the mapping a_k results in a new supergroup if and only if $a_k \notin \mathcal{D}$, Koch (1984). Otherwise, not only the group $\mathcal{H}$, but also the group $\mathcal{G}$ will be reproduced. Following Koch (1984), other supergroups $\mathcal{G}_k$ will be obtained by the coset decomposition $\mathcal{N}_{\mathcal{A}}(\mathcal{H}):\mathcal{D}$ of the group $\mathcal{N}_{\mathcal{A}}(\mathcal{H})$ relative to the group $\mathcal{D}$ and the transformation of $\mathcal{G}$ with the representatives of these cosets.
2. If there is a further minimal supergroup $\mathcal{G}_j \neq \mathcal{G}$ of the same index $[i]$, then $a_j \notin \mathcal{N}_{\mathcal{A}}(\mathcal{H})$, *i.e.* a_j is not an element of the affine normalizer of the group $\mathcal{H}$. How can such a mapping a_j be found?
   This mapping $a_j \in \mathcal{A}$ transforms the space group $\mathcal{G}$ onto the space group $\mathcal{G}_j = a_j^{-1}\mathcal{G}a_j$. Let $\mathcal{H}_j = a_j\mathcal{H}a_j^{-1}$ be obtained from $\mathcal{H}$ by the inverse of that transformation which transforms $\mathcal{G}$ to $\mathcal{G}_j$. Then the group $\mathcal{H}_j$ is a subgroup of $\mathcal{G}$ if and only if $\mathcal{H}$ is a subgroup of $\mathcal{G}_j$. Therefore, the transformation of $\mathcal{H}$ to $\mathcal{H}_j$ indicates the transforming element for the determination of the additional supergroup $\mathcal{G}_j$.
   If there is no subgroup $\mathcal{H}_j < \mathcal{G}$, then there is no other supergroup $\mathcal{G}_j$. If a subgroup $\mathcal{H}_j < \mathcal{G}$ exists, then also $\mathcal{G}_j$. Other minimal supergroups may be obtained from $\mathcal{G}_j$ again by considering the coset decomposition $\mathcal{N}_{\mathcal{A}}(\mathcal{H}):(\mathcal{N}_{\mathcal{A}}(\mathcal{H}) \cap \mathcal{N}_{\mathcal{A}}(\mathcal{G}_j))$ of the normalizer $\mathcal{N}_{\mathcal{A}}(\mathcal{H})$ relative to the intersection $(\mathcal{N}_{\mathcal{A}}(\mathcal{H}) \cap \mathcal{N}_{\mathcal{A}}(\mathcal{G}_j))$ in the same way as above.
   Summarizing: Any minimal supergroup of $\mathcal{H}$ may be found by transforming the group $\mathcal{H}$ onto all other subgroups $\mathcal{H}_j < \mathcal{G}$ of the same index, applying each time the inverse transformation to the group $\mathcal{G}$ for obtaining the group $\mathcal{G}_j$ and testing if $\mathcal{G}_j$ is already listed as a minimal supergroup of $\mathcal{H}$. If not, $\mathcal{G}_j$ is a new minimal supergroup of $\mathcal{H}$ and further minimal supergroups may be found by applying the coset decomposition of $\mathcal{N}_{\mathcal{A}}(\mathcal{H})$ relative to $(\mathcal{N}_{\mathcal{A}}(\mathcal{H}) \cap \mathcal{N}_{\mathcal{A}}(\mathcal{G}_j))$, as above.

The method for the determination of minimal supergroups can be generalized for the case of non-minimal supergroups $\mathcal{G}_j$ of $\mathcal{H}$. The main difference is that all distinct (non-maximal) subgroups $\mathcal{H}_j$ of $\mathcal{G}$ of a given index are not retrieved directly from the subgroup data of *IT*A1 but are calculated by a dedicated module of the program SUBGROUPGRAPH (*cf.* 3.1.1).

The programs

The Bilbao Crystallographic Server contains two programs related with supergroup-group pairs:

- MINSUP which gives all minimal supergroups of index 2, 3, and 4 of a given space group;
- SUPERGROUPS, which calculates all different supergroups of a given space-group type and a given index.

Input information

The program MINSUP needs as input the *IT*A number (or the Hermann-Mauguin symbol) of the group for which the minimal supergroups have to be determined.

The program returns a list with the minimal supergroups represented in a table which contains: the *IT*A number of the minimal supergroup, its Hermann-Mauguin symbol and the index of the group in the supergroup. There is also a link to the list with the transformation matrices that relate the basis of the supergroup with that of the subgroup.

The table described above contains only the types of the minimal supergroups. For the determination of all of the supergroups of a given type, it is necessary to select the type of the normalizers of the group and the supergroup. By default the Euclidean normalizers are used as listed in Table 15.3.2. of *IT*A. The user can also apply the affine normalizers listed in the same table. For a translation lattice with metrics of apparent higher symmetry the user may provide himself the set of additional generators for the specific Euclidean normalizer.

The program SUPERGROUPS takes as input the *IT*A-numbers of the space groups $\mathcal{G}$ and $\mathcal{H}$ and the index of $\mathcal{H}$ in $\mathcal{G}$. The transformation matrices relating the bases of $\mathcal{G}$ and $\mathcal{H}$ necessary for the determination of the supergroups $\mathcal{G}_j$ are retrieved from the *IT*A1 database. In case of a non-

minimal supergroup, the program SUBGROUPGRAPH determines the transformation matrix(ces) for the corresponding chains of maximal subgroups that relate $\mathcal{G}$ and $\mathcal{H}$. As in the case of MINSUP, the space-group normalizers used by default are the Euclidean normalizers. Also, there is a possibility for the user to use affine normalizers given in *IT*A, or to provide a specific one.

Output information

For the two supergroup programs, the result contains:

- The transformation matrix $(\boldsymbol{P}, \boldsymbol{p})_j$ that relates the basis of the supergroup with that of the subgroup.
- One representative from each coset in the decomposition of the supergroup $\mathcal{G}_j$ with respect to the group $\mathcal{H}$. The full cosets of the decomposition are also accessible. The coset decomposition is performed with respect to the basis of the subgroup $\mathcal{H}$.

URL of the program

http://www.cryst.ehu.es/cryst/supergroups.html

Remark 1. From the considerations given above it should have become clear that the aim of the presented procedure and the supergroup programs is to solve the following 'pure' group-theoretical problem: Given a group-subgroup pair of space groups, $\mathcal{G} > \mathcal{H}$, determine all supergroups $\mathcal{G}_j$ of $\mathcal{H}$, isomorphic to $\mathcal{G}$. The procedure does not include any preliminary checks on the compatibility of the metric of the studied space group, with that of a supergroup. Depending on the particular case some of the obtained supergroups are not space groups but just affine analogues of space groups (see Koch, 1984). As an example consider the cubic supergroups of $P2_12_12_1$: only if the three basis vectors of $P2_12_12_1$ have equal length one can speak of supergroups of the cubic $P2_13$ space-group type. However, for each group $P2_12_12_1$ there exist affine analogues of $P2_13$ as supergroups.

Remark 2. The number of supergroups of a space group $\mathcal{H}$ of a finite index is not always finite. This is the case of a space group $\mathcal{H}$ whose normalizer $\mathcal{N}(\mathcal{H})$ contains continuous translations in one, two or three independent directions (see *IT*A, Section 15). As typical examples one can consider the infinitely many centrosymmetrical supergroups of the polar groups: there are no restrictions on the location of the additional inversion centre on the polar axis. For such group-supergroup pairs there is a parameter *r*, *s* or/and *t* in the transformation matrix and in the translational part of the coset representatives. The parameters can have any value and each value corresponds to a different supergroup of the same space-group type.

Remark 3. The affine normalizers of triclinic and monoclinic groups are not isomorphic to groups of motions and they are not included in the normalizer database on the Bilbao Crystallographic Server. However, in the cases of groups with specialized metrics it is necessary to consider Euclidean normalizers of higher symmetry than for the general case (Koch & Müller, 1990).

3.2.1 Examples

- Case 1: Supergroups $\mathcal{G}_k = a_k^{-1}\mathcal{G}a_k$ of $\mathcal{H}$ with $a_k \in \mathcal{N}_{\mathcal{A}}(\mathcal{H})$.

Table 3. *P*422 supergroups of *P*222 $(a = b = c)$, index 2, as determined by MINSUP. The different supergroups are distinguished by the transformation matrices $(\boldsymbol{P}, \boldsymbol{p})_j$ and the coset representatives of the decomposition of $(P422)_j$ with respect to $\mathcal{H}$. (The unit element is taken as coset representative in all cases and is not listed). The location of the 4-fold axis is referred to the orthorhombic cell.

Supergroup	$(\boldsymbol{P}, \boldsymbol{p})_j$	Coset Rep.	4-fold location
$(P422)_1$	**a**, **b**, **c**; 0 0 0	$(4_z \mid 0\ 0\ 0)$	0 0 0
$(P422)_2$	**a**, **b**, **c**; $^1/_2$ 0 0	$(4_z \mid \bar{1}/_2\ ^1/_2\ 0)$	$\bar{1}/_2$ 0 0
$(P422)_3$	**b**, **c**, **a**; 0 0 0	$(4_y \mid 0\ 0\ 0)$	0 0 0
$(P422)_4$	**b**, **c**, **a**; 0 $^1/_2$ 0	$(4_y \mid \bar{1}/_2\ 0\ \bar{1}/_2)$	$\bar{1}/_2$ 0 0
$(P422)_5$	**c**, **a**, **b**; 0 0 0	$(4_x \mid 0\ 0\ 0)$	0 0 0
$(P422)_6$	**c**, **a**, **b**; $^1/_2$ 0 0	$(4_x \mid 0\ \bar{1}/_2\ ^1/_2)$	0 $\bar{1}/_2$ 0

As an example we consider the group-supergroup pair $\mathcal{H} < \mathcal{G}$ with $\mathcal{H} = P222$ (No. 16 in *IT*A) and the supergroup $\mathcal{G} = P422$ (No. 89 in *IT*A) of index $[i] = 2$. Further, we suppose that the group *P*222 has a specialized cell metrics specified as $(a = b = c)$.
In the subgroup data of *P*422 there is only one entry for the subgroup *P*222 of index 2. We are interested in all *P*422 supergroups of index 2 of the group *P*222. The affine normalizer of *P*422 coincides with its Euclidean normalizer and it has the translations $(x + ^1/_2, y + ^1/_2, z)$, $(x, y, z + ^1/_2)$ and the inversion as additional generators (*cf. IT*A, Table 15.2). The Euclidean normalizer of *P*222 with $a = b = c$ coincides with its affine normalizer. It corresponds to the cubic group $Pm\bar{3}m$ with the additional translations $(x + ^1/_2, y, z)$, $(x, y + ^1/_2, z)$ and $(x, y, z + ^1/_2)$. The decomposition of $\mathcal{N}(\mathcal{H})$ with respect to the intersection of the two normalizers contains 6 cosets, *i.e.* there are 6 supergroups of *P*222 isomorphic to *P*422. The different supergroups as calculated by MINSUP are listed in Table 3. They are distinguished by their transformation matrix-column pairs $(\boldsymbol{P}, \boldsymbol{p})_j$ and the coset representatives of the decomposition of $\mathcal{G}_j$ with respect to $\mathcal{H}$. The existence of the 6 different supergroups becomes obvious if we consider the type and location of the symmetry elements corresponding to the listed coset representatives of the different supergroups (Table 3). Due to the specialized metrics of *P*222 the four-fold axis of *P*422 can be chosen along any of the three orthorhombic axes. Accordingly, the 6 supergroups are distributed into three pairs. The

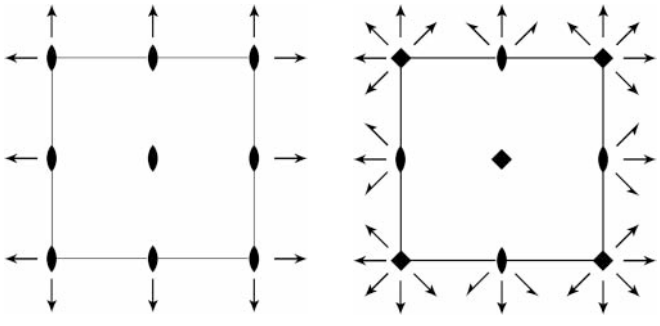

Fig. 6. Space-group diagrams for (a) *P*222 with specialized cell metrics (see the text), and (b) *P*422. For explanations, see *IT*A, Chapter 1.4.

comparison of the space-group diagrams of *P*422 and *P*222 (Fig. 6) shows that the two supergroups for each orientation of the four-fold axis correspond exactly to the two possible locations of the four-fold axis in the orthorhombic cell.

- Case 2: Supergroups $\mathcal{G}_k = a_k^{-1}\mathcal{G}\,a_k$ of $\mathcal{H}$ with $a_k \notin \mathcal{N}_{\mathcal{A}}(\mathcal{H})$.
  Consider the *Cmcm* minimal supergroups of *Pnma* (No. 62) of index 2. The group *Cmcm* (No. 63) has two maximal *Pnma* subgroups: $(Pnma)_1$ specified by $(\boldsymbol{P}, \boldsymbol{p})_1 = (\mathbf{b}, \mathbf{c}, \mathbf{a})$, and $(Pnma)_2$ with $(\boldsymbol{P}, \boldsymbol{p})_2 = (\mathbf{c}, \mathbf{a}, \mathbf{b}; {}^1/_4, {}^1/_4, 0)$. The Euclidean and affine normalizers of *Cmcm* and *Pnma* are identical and correspond to the group *Pmmm* with the additional translations $(x + {}^1/_2, y, z)$, $(x, y + {}^1/_2, z)$ and $(x, y, z + {}^1/_2)$. Accordingly, the application of the normalizer procedure to any of the two group-subgroup pairs will not generate further equivalent supergroups. The first pair $Cmcm > (Pnma)_1$ gives rise to the minimal supergroup $Bbmm(Cmcm)$. The second supergroup $Amma(Cmcm)$ can only be obtained considering the second group-subgroup pair. Both supergroups are related by a cyclic rotation of the three axes which is not in the normalizer of $\mathcal{H}$ (or $\mathcal{G}$).

3.3 Relations of Wyckoff positions for a group-subgroup pair of space groups

The problem

Consider group-subgroup related space groups $\mathcal{G} > \mathcal{H}$. Atoms which are symmetrically equivalent under $\mathcal{G}$, *i.e.* belong to the same orbit of $\mathcal{G}$, may become non-equivalent under $\mathcal{H}$, (*i.e.* the orbit splits) and/or their site symmetries may be reduced. The orbit relations induced by the symmetry reduction are the same for all orbits belonging to a Wyckoff position, so one can speak of Wyckoff-position relations or splitting of Wyckoff positions. Theoretical aspects of the relations of the Wyckoff positions for a group-subgroup pair of space groups $\mathcal{G} > \mathcal{H}$ have been treated in detail by Wondratschek (1993). A complete compilation of the Wyckoff-position splittings for all space groups and all their maximal subgroups is published in Part 3 of *IT*A1. A parameterized form of the relations describes the splittings for the infinite number of maximal isomorphic subgroups. However, for certain applications the published data are not sufficient: it is often necessary to have the appropriate tools for the calculations of the Wyckoff-position splittings for $\mathcal{G} > \mathcal{H}$ when $\mathcal{H}$ is not a maximal subgroup of $\mathcal{G}$, or when the space groups do not refer to conventional settings. The program WYCKSPLIT (Kroumova, Aroyo, Perez-Mato, 1998a) calculates the Wyckoff-position splittings for any group-subgroup pair. The space groups can be referred to conventional and non-conventional settings. In addition, the program provides the relations between the representatives of the orbit of $\mathcal{G}$ and the corresponding representatives of the suborbits of $\mathcal{H}$.

The method

The problem to be solved is the following: Given the group $\mathcal{G}$ and its subgroup $\mathcal{H}$ of index $[i]$, determine the splitting of a Wyckoff position $\mathcal{W}_{\mathcal{G}}$ of $\mathcal{G}$ into Wyckoff positions $\mathcal{W}_{\mathcal{H}}^j$ of the subgroup and the corresponding relations between the representatives. For simplifying the notation, we assume in the following that the group $\mathcal{G}$, its Wyckoff-position representatives, and the points of the orbits are referred to the basis of the subgroup.

1. Splitting of the General position
   Consider the group-subgroup chain of space groups $\mathcal{G} > \mathcal{H}$. It is possible to decompose $\mathcal{G}$ into right cosets with respect to $\mathcal{H}$:

$$\mathcal{G} = \mathcal{H} + \mathcal{H}g_2 + \ldots + \mathcal{H}g_i\,. \tag{3}$$

   The number of the $\mathcal{H}$-cosets equals the index of $\mathcal{H}$ in $\mathcal{G}$, and g_j, $j = 1, \ldots, i$, are the chosen coset representatives with g_1 equals the identity.
   The general-position orbits $\mathcal{O}_{\mathcal{G}}(X_0)$ have unique splitting schemes: they are split into $[i]$ suborbits $\mathcal{O}_{\mathcal{H}}(X_{0,j})$ of the general position of the subgroup, *i.e.* all are of the same multiplicity:

$$\mathcal{O}_{\mathcal{G}}(X_0) = \mathcal{O}_{\mathcal{H}}(X_{0,1}) \cup \ldots \cup \mathcal{O}_{\mathcal{H}}(X_{0,i})\,. \tag{4}$$

   This property is a direct corollary of the following lemma (Wondratschek, 1993):
   Let $\mathcal{G}$ be a space group and $\mathcal{H}$ a subgroup of index $[i]$ of $\mathcal{G}$. The site-symmetry groups of a point X under the space group $\mathcal{G}$, $S_{\mathcal{G}}(X)$ and under its subgroup $\mathcal{H}$, $S_{\mathcal{H}}(X)$, define the so-called reduction factors of the site symmetry: $R = \dfrac{|S_{\mathcal{G}}(X)|}{|S_{\mathcal{H}}(X)|}$. When the space-group symmetry is reduced from $\mathcal{G}$ to $\mathcal{H}$ and the orbit $\mathcal{O}_{\mathcal{G}}(X)$ of the point X in $\mathcal{G}$ splits into q orbits $\mathcal{O}_{\mathcal{H}}(X_j)$ of $\mathcal{H}$, the following relation holds:

$$[i] = \sum_{j=1}^{q} R_j\,. \tag{5}$$

   The maximal splitting corresponds to $R_j = 1$ for each $j = 1, \ldots, q$ and this is always the case if $\mathcal{O}_{\mathcal{G}}(X)$ is a general-position orbit.
   The determination of the splitting of the general-position orbit $\mathcal{O}_{\mathcal{G}}(X_0)$ is then reduced to the selection of the $[i]$ points $(X_{0,j})$ belonging to the $[i]$ independent suborbits $\mathcal{O}_{\mathcal{H}}(X_{0,j})$ of $\mathcal{H}$, Eq. (4). Due to the one-to-one mapping between the general-position points of $\mathcal{O}_{\mathcal{G}}(X_0)$ and the elements g of $\mathcal{G}$, the right cosets $\mathcal{H}g_k$ of the decomposition of $\mathcal{G}$ with respect to $\mathcal{H}$, Eq. (3), correspond to the suborbits $\mathcal{O}_{\mathcal{H}}(X_{0,j})$. In this way, the representatives of these cosets can be chosen as the $[i]$ points $X_{0,j}$ in the decomposition of $\mathcal{O}_{\mathcal{G}}(X_0)$.
2. Splitting of a special position
   The calculation of the splitting of a special Wyckoff position $\mathcal{W}_{\mathcal{G}}$ involves the following steps:
   - the determination of the suborbits $\mathcal{O}_{\mathcal{H}}(X_j)$ into which the special Wyckoff position orbit $\mathcal{O}_{\mathcal{G}}(X)$ has split;
   - the assignment of the orbits $\mathcal{O}_{\mathcal{H}}(X_j)$ to the Wyckoff positions $\mathcal{W}_{\mathcal{H}}^l$ of $\mathcal{H}$;
   - the determination of the correspondence between the points X_j^m of the suborbits $\mathcal{O}_{\mathcal{H}}(X_j)$ and the representatives of $\mathcal{W}_{\mathcal{H}}^l$.

The direct determination of the suborbits $\mathcal{O}_{\mathcal{H}}(X_j)$ is not an easy task. The restrictions on the site-symmetry groups $S_{\mathcal{H}}(X_j)$ which follow from the reduction-factor lemma, Eq. (5), are helpful but in many cases not sufficient for the determination of the suborbits. The solution used in our approach is based on the general-position decomposition, Eq. (4). It is important to note that each of the suborbits of the general position gives exactly one suborbit $\mathcal{O}_{\mathcal{H}}(X_j)$ when the variable parameters of $\mathcal{O}_{\mathcal{H}}(X_{0,j})$ are substituted by the corresponding parameters (fixed or variable) of the special position. The assignment of the suborbits to the Wyckoff positions of $\mathcal{H}$ is done by comparing the multiplicities of the orbits, the number of the variable parameters (the number of the variable parameters of $\mathcal{W}^l_{\mathcal{H}}$ is equal or greater than that of $\mathcal{O}_{\mathcal{H}}(X_j)$) and the values of the fixed parameters. If there is more than one Wyckoff position of $\mathcal{H}$ satisfying these conditions, then the assignment is done by a direct comparison of the points of the suborbit $\mathcal{O}_{\mathcal{H}}(X_j)$ with those of a special $\mathcal{W}^l_{\mathcal{H}}$ orbit obtained by substitution of the variable parameters by arbitrary numbers. The determination of the explicit correspondences between the points of $\mathcal{O}_{\mathcal{H}}(X_j)$ and the representatives of $\mathcal{W}^l_{\mathcal{H}}$ is done by comparing the values of the fixed parameters and the variable parameter relations in both sets.

3.3.1 The program

The program WYCKSPLIT calculates the splitting of the Wyckoff positions for a group-subgroup pair $\mathcal{G} > \mathcal{H}$, given the corresponding transformation relating the coordinate systems of $\mathcal{G}$ and $\mathcal{H}$.

Input information

The program needs as input the following information

- the sequential numbers of the space groups $\mathcal{G}$ and $\mathcal{H}$ as given in *IT*A which can be chosen from the list with the 230 space groups;
- the transformation matrix-column pair $(\boldsymbol{P}, \boldsymbol{p})$ that relates the basis of $\mathcal{G}$ to that of $\mathcal{H}$. The user can input a specific transformation or can be linked to the *IT*A1 database for the maximal subgroups of $\mathcal{G}$. In the case of a non-maximal subgroup, the program SUBGROUPGRAPH provides the transformation matrix(ces) for a specified index of $\mathcal{H}$ in $\mathcal{G}$. The transformations are checked for consistency with the conventional (default) settings of $\mathcal{G}$ and $\mathcal{H}$ used by the program.
- The Wyckoff positions $\mathcal{W}_{\mathcal{G}}$ to be split can be selected from a list. In addition, it is possible to calculate the splitting of any orbit $O_{\mathcal{G}}(X)$ specified by the coordinate triplet of one of its points.

Output information

- Splittings of the selected Wyckoff positions $\mathcal{W}_{\mathcal{G}}$ into Wyckoff positions $\mathcal{W}^l_{\mathcal{H}}$ of the subgroup, specified by their multiplicities and Wyckoff letters.
- The correspondence between the representatives of the Wyckoff position and the representatives of its suborbits is presented in a table where the coordinate triplets of the representatives of $\mathcal{W}_{\mathcal{G}}$ are referred to the bases of the group and of the subgroup.

WYCKSPLIT can treat group or subgroup data in unconventional settings, if the transformation matrices to the corresponding conventional settings are given.

URL of the program

http://www.cryst.ehu.es/cryst/wpsplit.html

3.3.2 Example

For illustrating the calculation of the Wyckoff-position splitting we consider the group-subgroup pair $P4_2/mnm > Cmmm$ of index 2, *cf.* Fig. 7. The relation between the conventional bases (**a**, **b**, **c**) of the group and of the subgroup (**a**′, **b**′, **c**′) is retrieved by the program MAXSUB and is given by: $\mathbf{a}' = \mathbf{a} - \mathbf{b}$, $\mathbf{b}' = \mathbf{a} + \mathbf{b}$, $\mathbf{c}' = \mathbf{c}$.

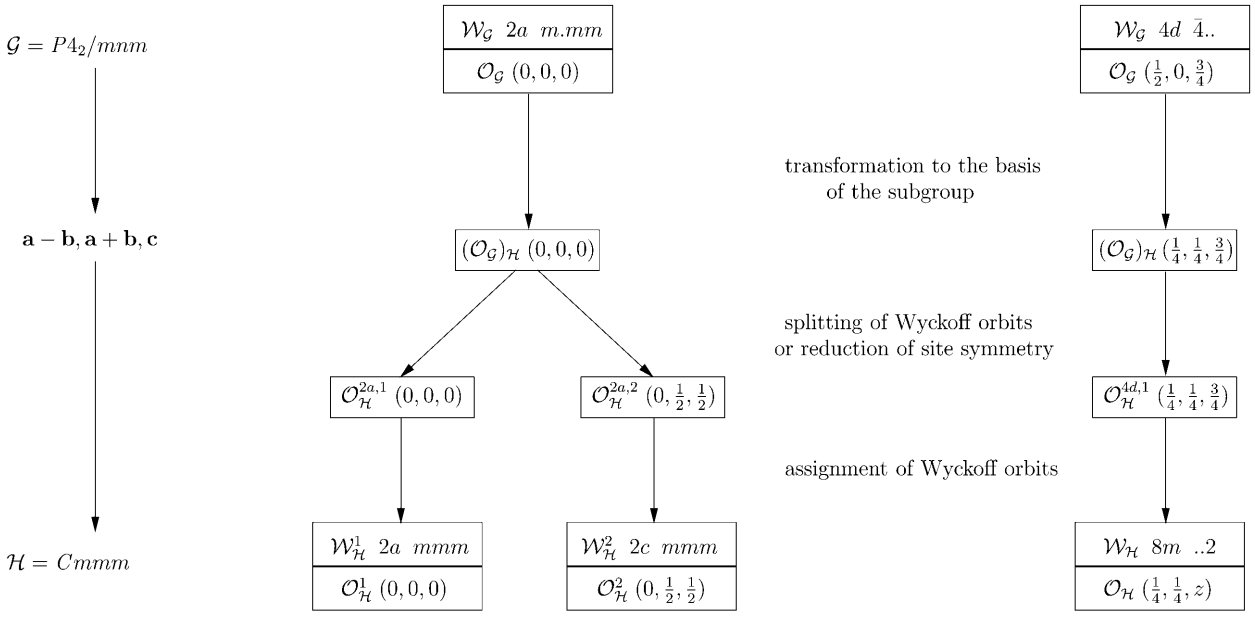

Fig. 7. Splitting of the Wyckoff positions 2*a m.mm* (0, 0, 0) and 4*d* $\bar{4}$.. ($^1/_2$, 0, $^3/_4$) of $P4_2/mnm$ with respect to its subgroup *Cmmm* of index 2. $(\mathcal{O}_{\mathcal{G}})_{\mathcal{H}}$ are the orbits of $P4_2/mnm$ in the basis of *Cmmm*.

Table 4. Wyckoff positions of *Cmmm* with multiplicity 2 and 8. Each Wyckoff position is specified by its multiplicity and Wyckoff letter (WP), site symmetry (SS) and a coordinate triplet of a representative element (Rep).

Orbits of mult. 2			Orbits of mult. 8		
WP	SS	Rep.	WP	SS	Rep.
2*d*	*mmm*	(0, 0, $^1/_2$)	8*q*	..*m*	(x, y, $^1/_2$)
2*c*	*mmm*	($^1/_2$, 0, $^1/_2$)	8*p*	..*m*	(x, y, 0)
2*b*	*mmm*	($^1/_2$, 0, 0)	8*o*	.*m*.	(x, 0, z)
2*a*	*mmm*	(0, 0, 0)	8*n*	*m*..	(0, y, z)
			8*m*	..2	($^1/_4$, $^1/_4$, z)

The general position of $P4_2/mnm$ splits into two suborbits of the general position of *Cmmm*:

$$16k\ 1\ (x,y,z) \rightarrow 16r\ 1(x,y,z) \cup 16r\ 1(x',y',z')\,.$$

This splitting is directly related to the coset decomposition of $P4_2/mnm$ with respect to *Cmmm*. As coset representatives, *i.e.* as points which determine the splitting of the general position one can chose $X_{0,1} = (x,y,z)$ and $X_{0,2} = (x',\ y',\ z') = (y,\ x + {}^1/_2,\ z + {}^1/_2)$ (referred to the basis of the subgroup).

The splitting of any special Wyckoff position is obtained from the splitting of the general position. The consecutive steps of the splittings of the special positions $4d\,\bar{4}\ldots({}^1/_2,\ 0,\ {}^3/_4)$ and $2a\ m.mm$ (0, 0, 0) are shown on Fig. 7. First it is necessary to transform the representatives of $\mathcal{W}_\mathcal{G}$ to the basis of $\mathcal{H}$ which gives the orbits $(\mathcal{O}_\mathcal{G})_\mathcal{H}$ (0, 0, 0) and $(\mathcal{O}_\mathcal{G})_\mathcal{H}$ ($^1/_4$, $^1/_4$, $^3/_4$). The substitution of the values $x = 0$, $y = 0$, $z = 0$ in the coordinate triplets of the decomposed general position of $\mathcal{G}$ (*cf.* the corresponding output of WYCKSPLIT) gives two suborbits of multiplicity 2 for the 2*a* position: $\mathcal{O}_\mathcal{H}^{2a,1}$ (0, 0, 0) and $\mathcal{O}_\mathcal{H}^{2a,2}$ (0, $^1/_2$, $^1/_2$). The assignment of the suborbits $\mathcal{O}_\mathcal{H}^{2a,j}$ to the Wyckoff positions of $\mathcal{H}$ (*cf.* Table 4) is straightforward. Summarizing: the Wyckoff position $2a\ m.mm$ (0, 0, 0) splits into two independent positions of *Cmmm* with no site-symmetry reduction:

$$2a\ m.mm\ (0,\ 0,\ 0) \rightarrow 2a\ mmm\ (0,\ 0,\ 0) \cup 2c\ mmm\ (0,\ {}^1/_2,\ {}^1/_2)\,.$$

No splitting occurs for the case of the special 4*d* position orbit: the result is one orbit of multiplicity 8, $\mathcal{O}_\mathcal{H}^{4d,1}$ ($^1/_4$, $^1/_4$, $^3/_4$). The assignment of $\mathcal{O}_\mathcal{H}^{4d,1}$ ($^1/_4$, $^1/_4$, $^3/_4$) is also obvious: there are 5 Wyckoff positions of *Cmmm* of multiplicity 8 but 4 of them are discarded as they have fixed parameters 0 or $^1/_2$ (Table 4). The orbit $\mathcal{O}_\mathcal{H}^{4d,1}$ belongs to the Wyckoff position $8m\,..2$ ($^1/_4$, $^1/_4$, z).

As expected the sum of the site-symmetry reduction factors equals the index of *Cmmm* in $P4_2/mnm$, Eq. (5), for both cases. The loss of the four-fold inversion axis results in the appearance of an additional degree of freedom corresponding to the variable parameter of $8m\,..2$ ($^1/_4$, $^1/_4$, z).

4. Conclusions

The *Bilbao Crystallographic Server* is a web site with crystallographic databases and programs available on-line. It has been operating for almost six years and new applications are being added regularly. The databases and the programs can be accessed through the main page of the server (www.cryst.ehu.es) and can be used free of charge with any web browser.

The server is built on a core of databases and the accompanying software is divided into several shells according to different topics. In this article we have provided a description of the set of databases available on the server and the shell formed by crystallographic computing programs. The utility of the applications is demonstrated by illustrative examples. The rest of the programs on the server, related to representations of space groups and point groups, and the applications facilitating the study of specific problems of solid-state physics and structural chemistry are the subject of a forthcoming article.

The databases of the Bilbao Crystallographic server include different space-group data: generators and general positions, Wyckoff positions, maximal subgroups of indices 2, 3, and 4, **k**-vector types, *etc*. Recently, we have started with the development of a database of subperiodic groups. The data are accessed through simple retrieval tools. In addition, as a part of the server one can find the database on incommensurate crystal structures, which provides the users with a web-interface for the search of a specific structure or the input of new structures.

The programs that combine the crystallographic data with group-theoretical algorithms form the second main shell of the server: 'Crystallographic computing programs'. It contains applications which are essential for problems related to group-subgroup relations between space groups including subgroups and supergroups of space groups, graphs of maximal subgroups for group-subgroup pairs, Wyckoff-position splitting schemes during symmetry reduction, *etc*.

The programs on the Bilbao Crystallographic server have user-friendly interfaces with links to documentation and on-line help for each of the consecutive steps in a calculation. One of the important advantages of the server is that the different programs can communicate with each other, so that the output of some programs is used directly as input data to others. In this way the Bilbao Crystallographic Server has turned into a working environment with the appropriate tools for treating problems of theoretical crystallography, solid-state physics and crystal chemistry.

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