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Crystallography online: Bilbao Crystallographic Server

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The *Bilbao Crystallographic Server* is a web site with crystallographic databases and programs available online (www.cryst.ehu.es). It has been operating for more than ten 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 server gives access to general information related to crystallographic symmetry groups (generators, general and special positions, maximal subgroups, Brillouin zones, etc.). Apart from the simple tools for retrieving the stored data, there are programs for the analysis of group-subgroup relations between space groups. There are also software package studying specific problems of solid-state physics, structural chemistry and crystallography.

Key words: Bilbao Crystallographic Server, crystallographic symmetry, online tools.

1. INTRODUCTION

The *Bilbao Crystallographic Server* is a web site with crystallographic databases and programs available online. The server has been operating since 1998, and new programs and applications are being added regularly [23, 2, 3]. 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 *Bilbao Crystallographic Server* is accessible at www.cryst.ehu.es.

The server is built on a database core, and contains different shells. The set of databases includes data from *International Tables for Crystallography*, Vol. A: Space-group symmetry (hereafter referred to as *IT*A)[12], and the data on maximal subgroups of space groups as listed in Part 1 of *International Tables for Crystallography*, Vol. A1: Symmetry relations between space groups (hereafter referred to as *IT*A1)[13]. There is an access to the crystallographic data for the subperiodic layer and rod groups (*International Tables for Crystallography*, Vol. E: Subperiodic groups [14]) and their maximal subgroups. A database on incommensurate structures incorporating modulated structures and composites, and a **k**-vector database with Brillouin-zone figures and classification tables of the wave vectors for all space groups are also available.

The innermost shell is formed by simple retrieval tools which serve as an interface to the databases. They allow the access to the information on space groups or subperiodic groups in different types of formats: HTML, text ASCII or XML. The second shell contains applications which are essential for problems involving group-subgroup related space groups $G > H$ (supergroups of space groups, chains of maximal subgroups relating G and H, splittings of Wyckoff positions for group-subgroup pairs). Then, follows a shell with programs on representations of point and space groups including the computation of spacegroup representations, their correlations for $G > H$, etc. Parallel to the crystallographic software a shell with programs facilitating the study of specific problems related to solid-state physics, structural chemistry and crystallography is also developed. For example, the program PSEUDO provides an online tool for systematic pseudosymmetry search based on group-subgroup relations between space groups. The detection of pseudosymmetry can be very useful in predicting phase transitions, including the identification of ferroic materials or the detection of false symmetry assignments in crystal structure determination [11, 21, 22]. The performance and efficiency of the program has been greatly improved by including a powerful cross-check of Wyckoff compatibility relations of the possible high-symmetry structures [9]. The automatic symmetry-mode analysis done by AMPLIMODES can be very useful for establishing the driving mechanisms of structural phase transi-

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tions or the fundamental instabilities at the origin of the distorted phases [25, 26]. Given the high- and the low-symmetry structure the program determines the atomic displacements that relate them, defines a basis of symmetry-adapted modes, and calculates the amplitudes and polarization vectors of the distortion modes of different symmetry frozen in the structure. In that shell one can also find a computer program that calculates the phonon extinction rules for inelastic neutron scattering experiments. Given the space group and the phonon symmetry specified by the wave vector, NEUTRON [17] examines the inelastic neutron scattering activity of the corresponding phonons for all possible types of scattering vectors. The systematic selection rules are also useful in the interpretation of the results of thermal diffuse scattering.

The aim of the present contribution is to report on the different databases and basic programs of the server related to the crystallographic groups, their group-subgroup relations and representations. Part of these databases and programs have been already described in [2, 3], and here we follow closely these presentations. They are completed by the description of the new developments until 2010. The presentation of the relevant databases and retrieval tools that access the stored crystallographic symmetry information is given in Section 2. The discussion of the accompanying applications related to group-subgroup and group-supergroup relations between space groups can be found in Section 3. The Section 4 introduces the basic programs for representations of crystallographic groups available on the Bilbao Crystallographic Server.

2. SPACE-GROUPS DATABASES AND RETRIEVAL TOOLS

The databases form the core of the Bilbao Crystallographic Server and the stored information is used by all computer programs available on the server. The space-group database includes information on the following symmetry items: generators and representatives of the general position of each space group specified by its *IT*A number and Hermann-Mauguin symbol; special Wyckoff positions including the Wyckoff letter, Wyckoff multiplicity, the site-symmetry group and the set of coset representatives, as given in *IT*A; the Reflection conditions including the general and special conditions. The programs and databases of the Bilbao Crystallographic Server use specific settings of space groups (hereafter referred to as standard or default settings) that coincide with the conventional space-group descriptions found in *IT*A. For space groups with more than one description in *IT*A, the following settings are chosen as standard: unique axis b setting, cell choice 1 for monoclinic groups, hexagonal axes setting for rhombohedral groups, and origin choice 2 (origin in $\bar{1}$) for the centrosymmetric groups listed with respect to two origins in *IT*A. The data from the databases can be accessed using the simple retrieval tools that use as input the number of the space group (*IT*A numbers). There is also a possibility to select the group from a table with *IT*A numbers and Hermann-Mauguin symbols. The output of the program 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 Wyckoff-position representatives for the non-standard settings of the space groups are specified by the transformed coordinates of the representatives of the corresponding default settings. The program NORMALIZER gives access to the data on the Euclidean and affine normalizers of space groups (*cf.* Part 15 of *IT*A) specified by a set of coset representatives of their decomposition with respect to the space groups. The assignments of the Wyckoff positions to Wyckoff sets are retrieved by the program WYCKSETS (*cf.* Table 14.2.3.2 of *IT*A).

2.1. Database on maximal subgroups

All maximal non-isomorphic subgroups and maximal isomorphic subgroups of indices 2, 3 and 4 of each space group can be retrieved from the database using the program MAXSUB[1]. Each subgroup H is specified by its *IT*A number, the index in the group G and the transformation matrix-column pair (P, p) that relates the default bases $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$ of H and $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ of G:

$$(\mathbf{a}', \mathbf{b}', \mathbf{c}') = (\mathbf{a}, \mathbf{b}, \mathbf{c})\, \boldsymbol{P} \qquad (2.1.1)$$

The column $\boldsymbol{p} = (p_1, p_2, p_3)$ of coordinates of the origin O_H of H is referred to the coordinate system of G.

The different maximal subgroups are distributed in classes of conjugate subgroups. For certain applications it is necessary to represent the subgroups H as subsets of the elements of G.This is achieved by an option in MAXSUB which transforms the gener-

[1] A subgroup $H < G$ is maximal if no subgroup Z exists for which $H < Z < G$ holds.

al-position representatives of H by the corresponding matrix-column pair $(\boldsymbol{P}, \boldsymbol{p})^{-1}$ to the coordinate system of G. A link provides the splittings of all Wyckoff positions of G with respect to those of H.

Maximal subgroups of index higher than 4 have indices p, p^2 or p^3, where p is a prime. They are isomorphic subgroups and are infinite in number. In *IT*A1 the isomorphic subgroups are listed not individually but as members of series under the heading 'Series of maximal isomorphic subgroups'. The program SERIES provides the access to the database of maximal isomorphic subgroups of the *Bilbao Crystallographic Server*. Apart from the parametric *IT*A1 descriptions of the series, its output provides the individual listings of all maximal isomorphic subgroups of indices as high as 27 for all space groups except for the cubic ones where the index is 125. The format and content of the subgroup data are similar to those of MAXSUB access tool. In addition, there is a special tool (under 'define a maximal index' on the SERIES web form) that permits the online generation of maximal isomorphic subgroups of any index up to 131 for all space groups. (Note that these data are only online generated and do not form part of the (static) database on isomorphic subgroups.)

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 for Crystallography* Vol. E: Subperiodic Groups [14]. For the moment the *Bilbao Crystallographic Server* provides a free online access to a database for the layer and rod 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 [5] and rod groups 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. Brillouin zones and wave-vectors classification

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 [27], see also [4]. 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 wave 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 the wave vector follows from the multiplicity of the Wyckoff position.
- All wave-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 [10] (hereafter referred to as CDML). The retrieval tool KVEC of the k-vector database uses 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 coordinates as listed in CDML. 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. The wave-vector coordinates of CDML refer always to primitive basis irrespective whether the conventional description of the space group is with respect to a centred or primitive basis. For that reason, in the case of space groups with centred lattices the wave-vector coordinates with respect to a basis that is dual to the conventional basis in direct space are also included in the tables. (For space groups with primitive lattices, the wave-vector coordinates referred to a primitive basis coincide with those referred to the dual basis.)

An additional tool allows the complete characterization of any wave vector of the reciprocal space (not restricted to the first Brillouin zone): given the **k**-vector coordinates referred either to primitive (CDML) or conventional dual basis, the program assigns the **k**-vector to the corresponding wave-vector symmetry type, specifies its CDML label, calculates the little co-group and the arms of the **k**-vector stars. 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.

Example: Brillouin zones and special k-vectors of the arithmetic crystal class $\bar{4}m2I$. The following example illustrates the relation between the traditional and the reciprocal-space group descriptions of the wave-vector types of space-group irreps. The included figures and tables form part of the output of the access tool KVEC.

The are two space groups belonging to the arithmetic crystal class $\bar{4}m2I$: $I\bar{4}m2 - D_{2d}^{9}(119)$ and $I\bar{4}c2 - D_{2d}^{10}(120)$. The **k**-vector types of that arithmetic crystal class are described with respect to the corresponding reciprocal space group which is isomorphic to $I\bar{4}2m(121)$. Depending on the relations between the lattice constants *a*, *b* and *c*, there are two topologically different bodies of the Brillouin

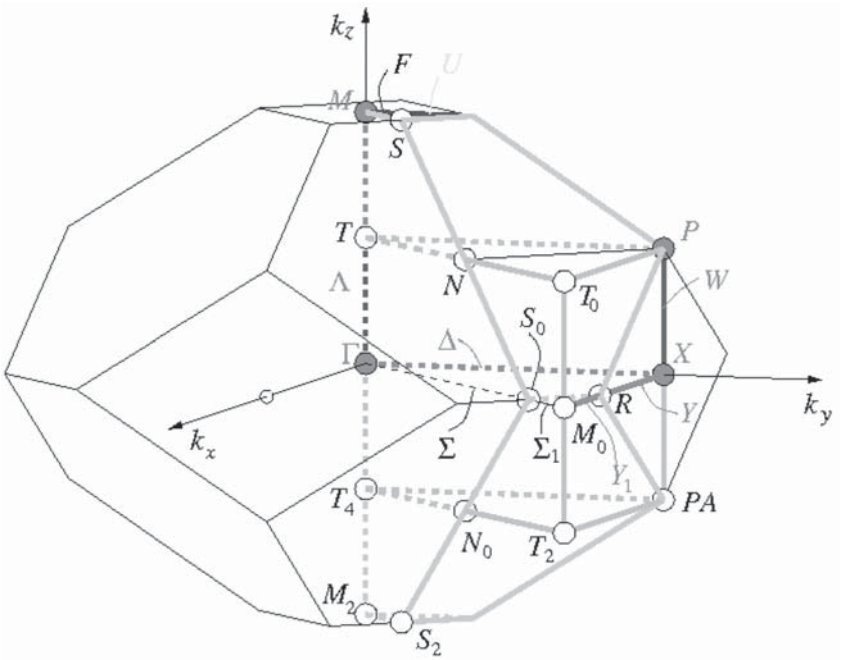


Fig. 1. Brillouin zone, asymmetric unit and representation domain of CDML for the arithmetic crystal class $\bar{4}m2I$: $c > a$: space groups $I\bar{4}m2 - D_{2d}^{9}(119)$ and $I\bar{4}m2 - D_{2d}^{10}(120)$; reciprocal-space group $I\bar{4}2m^*$, No. 121: $c^* < a^*$. The representation domain of CDML is different from the asymmetric unit.

zone displayed in Fig. 1 and Fig. 2 by thin black lines; the first one has 24 vertices, 48 lines and 14 faces, the other has 18 vertices, 28 lines 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 of CDML are more complicated than the asymmetric units of *IT*A, see Fig. 1 and Fig. 2.

The representatives of the **k**-vectors symmetry points or of symmetry lines, as well as the edges of the representation domain of CDML and of the chosen asymmetric unit are brought out in colors. A **k**-vectors symmetry point is designated by a red or cyan if it belongs to the asymmetric unit or to the representation domain of CDML. Points listed by CDML are not colored if they are part of a symmetry line or symmetry plane only. The color of the line is pink for an edge of the asymmetric unit which is not a symmetry line and it is red for a symmetry line of the asymmetric unit. The color of the line is brown with the name in red for a line which is a symmetry line as well as an edge of the asymmetric unit. The edges of the representation domains of CDML (displayed in the same figure) are colored in light blue. The corresponding symmetry points and lines are colored cyan. Edges of the representation domain or common edges of the representation domain and the asymmetric unit are colored dark blue with the letters in cyan if they are symmetry lines of the representation domain but not of the asymmetric unit. To save space we have included only part of the list of k-vector relations for the arithmetic class $\bar{4}m2I$ in the table shown in Fig. 3 (a screen-shot of the output of the access tool KVEC), corresponding to Fig. 1. The **k**-vector parameters of CDML (second column) of the table in Fig. 3 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. The parameter ranges (last column) are chosen such that each k-vector orbit is represented exactly once.

One takes from the table given in Fig. 3 that different k labels of CDML (first column) may correspond to the same Wyckoff position may belong to the same type of **k** vectors, *i. e.* may belong to the same type of **k** and 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 8 *i* (..m) (fourth column) is split into two parts, *SM* and *F*. In the *IT*A description $SM \cup F$ corresponds to one line $[GMM_0]$, $(x, x, 0)$, with $0 < x < 1/2$. The splitting of the 8 *i* 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 *SM* is not split.

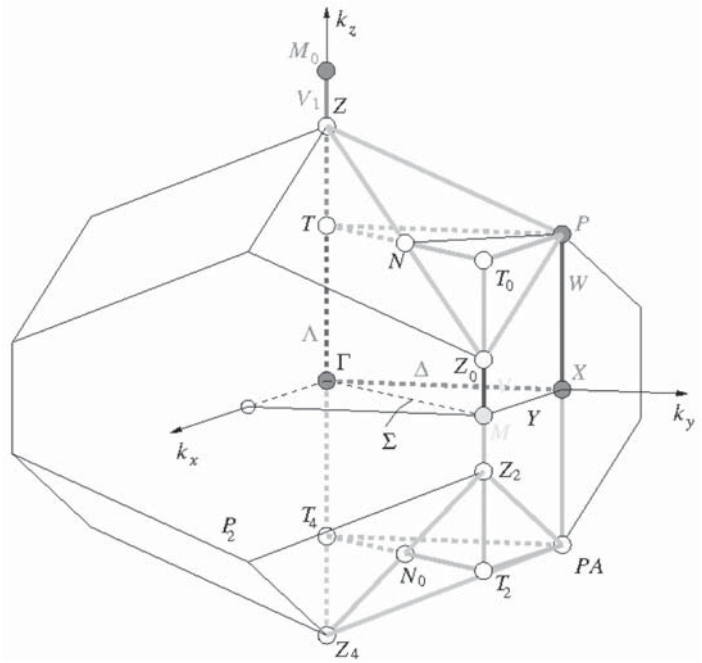


Fig. 2. Brillouin zone, asymmetric unit and representation domain of CDML for the arithmetic crystal $\bar{4}m2I$: $c < a$: space groups $I\bar{4}m2 - D_{2d}^{9}(119)$ and $I\bar{4}c2 - D_{2d}^{10}(120)$; reciprocal-space group $I\bar{4}2m^*$, No. 121: $c^* > a^*$. The representation domain of CDML is different from the asymmetric unit.

k-vector description			Wyckoff Position			ITA description
CDML*		Conventional-ITA	ITA			Coordinates
Label	Primitive					
GM	0,0,0	0,0,0	a	2	-42m	0,0,0
M	1/2,1/2,-1/2	0,0,1	b	2	-42m	0,0,1/2
X	0,0,1/2	1/2,1/2,0	c	4	222.	0,1/2,0
P	1/4,1/4,1/4	1/2,1/2,1/2	d	4	-4..	0,1/2,1/4
LD	u,u,-u	0,0,2u	e	4	2.mm	0,0,z : 0 < z < 1/2
DT	0,0,u	u,u,0	f	8	.2.	0,y,0 : 0 < y < 1/2
Y	-u,u,1/2 ex	1/2+u,1/2-u,0	g	8	.2.	x,1/2,0 : 0 < x <= r
U	1/2,1/2,-1/2+u ex	u,u,1	g	8	.2.	0,y,1/2 : 0 < y < g=1/2-r
U~Y_1=[R M_0]			g	8	.2.	x,1/2,0 : r < x < 1/2
Y+Y_1			g	8	.2.	x,1/2,0 : 0 < x < 1/2
W	u,u,1/2-u	1/2,1/2,2u	h	8	2..	0,1/2,z : 0 < z < 1/4
N	0,1/2,0 ex	1/2,0,1/2	i	8	..m	1/4,1/4,1/4
SM	-u,u,u ex	2u,0,0	i	8	..m	x,x,0 : 0 < x <= s_1
F	1/2-u,1/2+u,-1/2+u ex	2u,0,1	i	8	..m	x,x,1/2 : 0 < x < s=1/2-s_1
F~SM_1=[S_0 M_0]			i	8	..m	x,x,0 : s_1 < x < 1/2
SM+SM_1=[GM M_0] ex			i	8	..m	x,x,0 : 0 < x < 1/2

Fig. 3. List of **k**-vector symmetry types (selection) for the arithmetic crystal class $\bar{4}m2I$: $c > a$: space groups $I\bar{4}m2 - D_{2d}^{9}(119)$ and $I\bar{4}c2 - D_{2d}^{10}(120)$; reciprocal-space group $I\bar{4}2m^{*}$, No. 121 (*cf.* Fig. 1).

3. GROUP-SUBGROUP RELATIONS OF SPACE GROUPS

3.1. Subgroups of space groups

If two space groups G and H form a group–subgroup pair $G > H$, it is always possible to represent their relation by a chain of intermediate maximal subgroups Z_k: $G > Z_1 > \cdots > Z_n = H$. For a specified index of H in G there are, in general, a number of possible chains relating both groups, and a number of different subgroups $H_j < G$ isomorphic to H. We have developed two basic tools for the analysis of the group–subgroup relations between space groups: SUBGROUPGRAPH [15], and HERMANN [8]. Given the space-group types G and H, and an index [i], both programs determine all different subgroups H_j of G with the given index, and their distribution into classes of conjugate subgroups with respect to G. Due to its importance in a number of group–subgroup problems, the program COSETS is included as an independent application. It performs the decomposition of a space group in cosets with respect to one of its subgroups. Apart from these basic tools, there are two complementary programs which are useful in specific crystallographic problems that involve group–subgroup relations between space groups. The program CELLSUB calculates the subgroups of a space group for a given multiple of the unit cell. The common subgroups of two or three space groups are calculated by the program COMMONSUBS. In the following we will consider in more details the program SUBGROUPGRAPH which is the main program for the study of the group-subgroup relations between space groups. For a description of the rest of the programs of the group-subgroup shell the reader is referred to Ref. [2].

3.1.1. The program SUBGROUPGRAPH

The program is based on the data for the maximal non-isomorphic subgroups of index 2, 3 and 4 and isomorphic subgroups of indices up to 9 of the space groups. 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.

The specification of the group–subgroup pair $G > H$ leads to a reduction of the total graph to a subgraph with G as the top vertex and H as the bottom vertex, see the example at the end of this subsection. In addition, the $G > H$ subgraph, referred to as the general $G > H$ graph, contains all possible groups Z_k which appear as intermediate maximal

subgroups between G and H. It is important to note that in the general $G > H$ 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 have to be distinguished from the *complete* graphs where all space groups occurring in a group–subgroup graph are indicated by different space-group nodes.

The number of the vertices in the general $G > H$ graph may be further reduced if the index of H in G is specified. The obtained subgraph is again of contracted type. For the cases of specified indices, the program SUBGROUPGRAPH produces also complete graphs that are equal for subgroups of a conjugacy class; the different orientations and/or origin shifts of the conjugate subgroups Hs are manifested by the different transformation matrices $(\boldsymbol{P}, \boldsymbol{p})_s$ listed by the program.

Input Information

- The space groups G and H can be introduced by their *IT*A numbers or by their Hermann-Mauguin symbols chosen from a list provided by the program.
- The index of H in G is optional.

Output Information

- Group-subgroup pair $G > H$ with non-specified index.

1. The list of the possible intermediate space groups Z_k relating G and H.

2. A contracted graph.

Each space-group type in the list corresponds to one node in the graph, and the maximal subgroups are the neighbors (successors) of this node. Group–subgroup relations occurring in both directions are represented by nodes connected by two lines with opposite arrows. Maximal isomorphic subgroups are shown by loop edges (nodes connected to themselves), *cf*. Fig. 4.

- Group-subgroup pair $G > H$ with specified index

1. A list with all possible chains of maximal subgroups relating G and H with this index. (The program has no access to the data on maximal isomorphic subgroups with indices higher than 9).

2. The graphical representation.

The graphical representation contains the intermediate groups that connect G and 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.

For a given index of H in G, the different subgroups H_j of that index are calculated and distributed into classes of conjugate subgroups of G. The subgroups of a conjugacy class form a block where each subgroup is specified by the corresponding transformation matrix-column pair $(\boldsymbol{P}, \boldsymbol{p})_j$ that relates the default bases of G and H_j. There is also a link to a list of the elements of the subgroups transformed to the basis of the group G, which allows the identification of those elements of G that are retained in the subgroup. The list of transformation

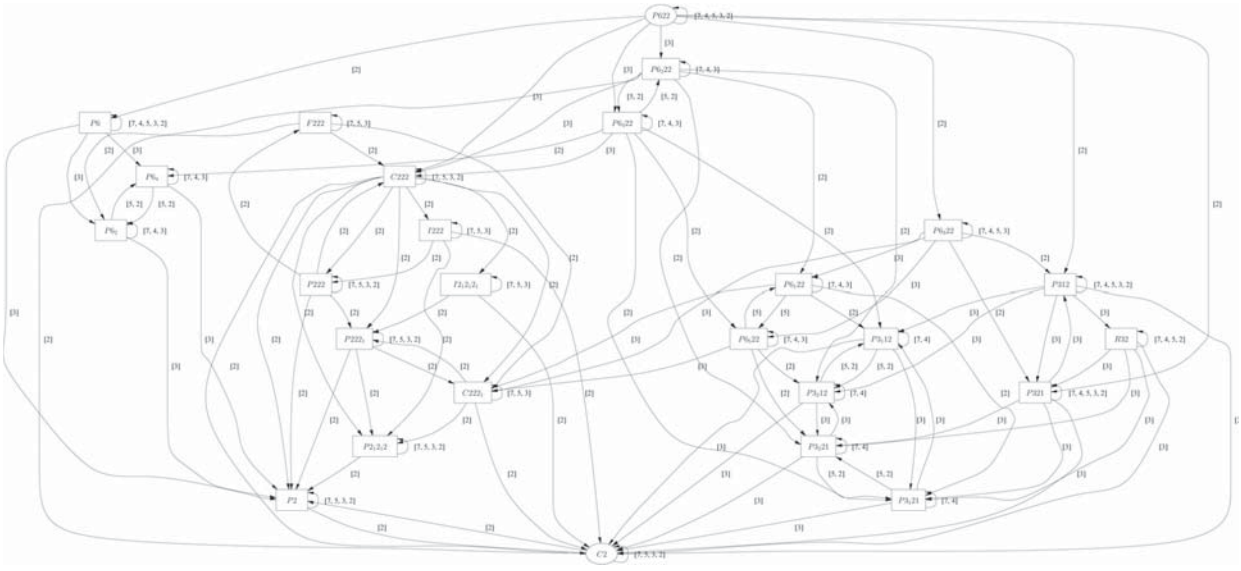


Fig. 4. General contracted graph for $P622$ (No. 177) > $C2$ (No. 5) as given by the program SUBGROUPGRAPH. The nodes of the graph correspond to the space-group types that can appear as intermediate groups in the chain of the group-subgroup pair $P622 > P2$. Each edge of the graph corresponds to a maximal subgroup pair of the indicated index [i]. Isomorphic subgroups (of indices up to 7) are shown as loops.

matrices that give the same (identical) subgroup is accessible under a separate link (*cf*. Fig. 7).

The graph contains the intermediate space groups Z_k for the pair $G \overset{i}{>} H$ but contrary to the graph of the previous step, the different isomorphic subgroups are represented by different nodes, *i.e*. the graph is a complete one. All isomorphic subgroups H_j are given at the bottom of the graph. Their labels are formed by the symbol of the subgroup followed by a number given in parenthesis which specifies the class of conjugate subgroups to which the subgroup 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 H_j can be very complicated and difficult to overview. Alternatively, a more simple graph associated to a single specific subgroup H_j (identical for all subgroups within a conjugacy class) can also be obtained.

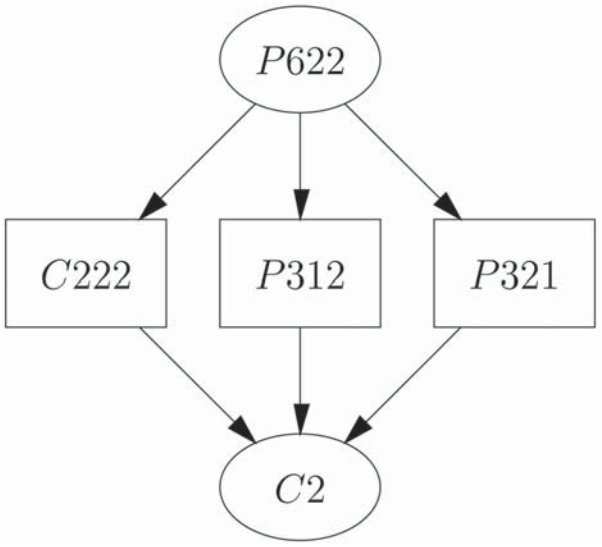


Fig. 5. Contracted graph for *P*622 (No. 177) > *C*2 (No. 5), index 6, as given by the program SUBGROUPGRAPH. The nodes of the graph correspond to space-group types. Each edge of the graph corresponds to a maximal subgroup pair.

Example: Consider the group–subgroup relations between the groups *G* = *P*622, No. 177, and *H* = *C*2, No. 5. If no index is specified then the graph of maximal subgroups that relates *P*622 and *C*2 is represented as a table indicating the space-group types of the possible intermediate space groups Z_k, and the corresponding indices. The contracted general *P*622 > *C*2 graph is shown in Fig. 4. Two edges with opposite arrows between a group–subgroup pair correspond to group–subgroup relations in both directions, *e.g*., the pair *P*62 and *P*64. 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. 5 the contracted graph *P*622 > *C*2 of index 6 is shown. The data in Fig. 7 and the complete graph shown in Fig. 6 indicate that there are six different *C*2 subgroups of *P*622 > *C*2 of index 6, distributed in two classes of conjugate subgroups. One of the conjugacy classes consists of the three different subgroups of space-group type *C*2 whose twofold axes point along $[1\bar{1}0]$, [120] and $[\bar{2}\bar{1}0]$ of *P*622. The other three subgroups with two-fold axes along [100], [010] and $[\bar{1}\bar{1}0]$ of *P*622 give rise to the second class of conjugate subgroups. The cor-

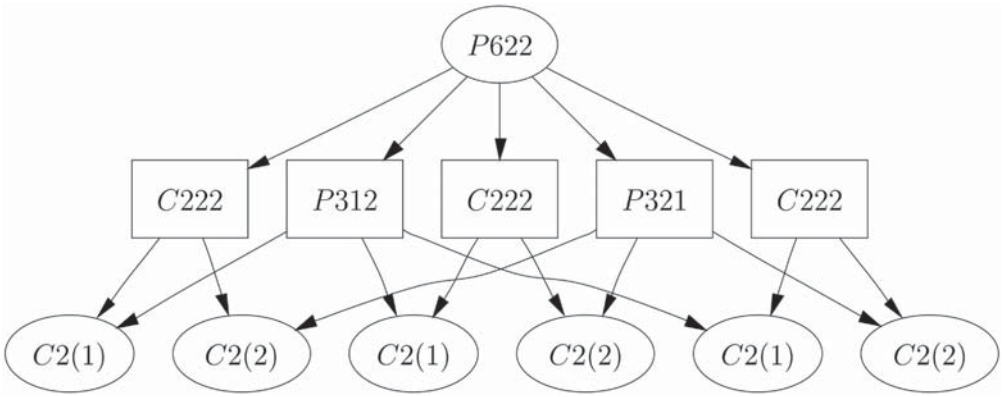
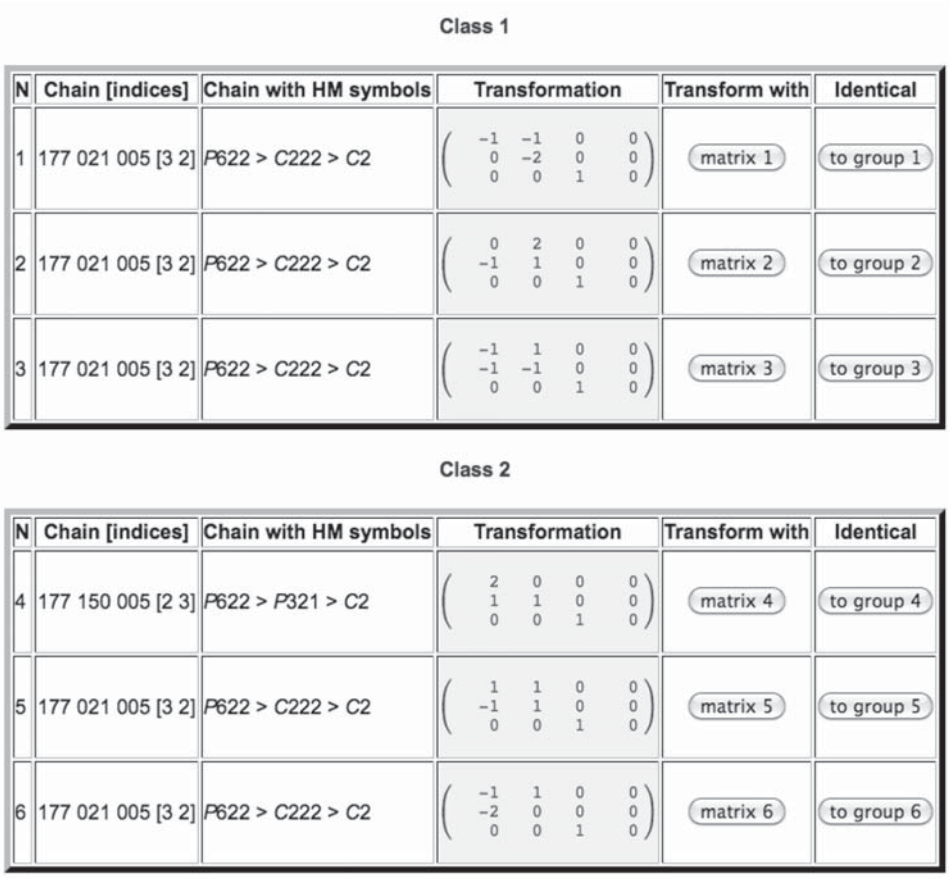


Fig. 6. Complete graph for *P*622 (No. 177) > *C*2 (No. 5), index 6, as given by the program SUBGROUPGRAPH. The nodes represent space groups and not space-groups types. The six subgroups of the type *C*2 are distributed into two classes of conjugate subgroups which are indicated in the parentheses after the space-group symbol. The three subgroups *C*2(1) with twofold axes along $[1\bar{1}0]$, [120] and $[\bar{2}\bar{1}0]$ of *P*622 belong to the same conjugacy class. They have equal complete single graphs, which differ from the graph of the subgroups *C*2(2) of the second conjugacy class. The latter corresponds to subgroups whose twofold axes point along [100], [010] and $[\bar{1}\bar{1}0]$ of *P*622.



Class 1

N	Chain [indices]	Chain with HM symbols	Transformation	Transform with	Identical
1	177 021 005 [3 2]	*P*622 > *C*222 > *C*2	$\begin{pmatrix} -1 & -1 & 0 & 0 \\ 0 & -2 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	matrix 1	to group 1
2	177 021 005 [3 2]	*P*622 > *C*222 > *C*2	$\begin{pmatrix} 0 & 2 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	matrix 2	to group 2
3	177 021 005 [3 2]	*P*622 > *C*222 > *C*2	$\begin{pmatrix} -1 & 1 & 0 & 0 \\ -1 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	matrix 3	to group 3

Class 2

N	Chain [indices]	Chain with HM symbols	Transformation	Transform with	Identical
4	177 150 005 [2 3]	*P*622 > *P*321 > *C*2	$\begin{pmatrix} 2 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	matrix 4	to group 4
5	177 021 005 [3 2]	*P*622 > *C*222 > *C*2	$\begin{pmatrix} 1 & 1 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	matrix 5	to group 5
6	177 021 005 [3 2]	*P*622 > *C*222 > *C*2	$\begin{pmatrix} -1 & 1 & 0 & 0 \\ -2 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	matrix 6	to group 6

Fig. 7. Screen-shot of the list of the six subgroups *C*2 (No. 5) of *P*622 (No. 177), index 6, as given by the program SUBGROUPGRAPH. The subgroups $(C2)_j$, $j = 1, \ldots, 6$ are distributed in two conjugacy classes and each subgroup is specified by its transformation matrix $(\boldsymbol{P}, \boldsymbol{p})_j$.

responding transformations can be read from the screen-shot table shown in Fig. 7. (Note that the standard setting for *C*2 is the UNIQUE AXIS *b* setting.) The complete graph *P*622 > *C*2, index 6 (Fig. 6), also shows that there are two different maximal subgroup chains to each subgroup *C*2. The subgroups of a conjugacy class have the same complete single graphs, while the complete graphs of subgroups of different conjugacy classes differ in general.

3.2. Supergroups of space groups

The problem of the determination of the supergroups of a given space group is of rather general interest. For several applications it is not sufficient to know only the space-group types of the supergroups of a given group; it is necessary to have available all different supergroups $G_r > H$ which are isomorphic to *G*, and are of the same index [*i*]. In the literature there are few papers treating the supergroups of space groups in detail [18, 29]. 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 *H* the list of those space-group types in which *H* occurs as a maximal subgroup (*cf.* Section 2.1). It is not trivial to determine all supergroups $G_r > H$ if only the types of the minimal supergroups are known. The Bilbao Crystallographic Server offers two basic programs [16] that solve that problem for a given finite index [*i*]: (i) the program MINSUP, which gives all minimal supergroups of indices 2, 3, 4, 5, 7 and 9 of a given space group; and (ii) the program SUPERGROUPS, which calculates all different supergroups of a given space-group type and a given index. Similar to the case of subgroups, we have developed two complementary programs that involve the calculation of supergroups of space groups. The program CELLSUPER calculates the supergroups of a space group for a given $[i_L]$ index, while the program COMMONSUPER is for the computation of common supergroups of two or more space groups.

The following discussion concerns the two basic programs MINSUP and SUPERGROUPS. For details on the complementary programs for group-su-

pergroup relations between space groups the reader is referred to Ref. [2].

3.2.1. The programs MINSUP and SUPERGROUPS

The determination of all supergroups G_r of a given space-group type G and an index [i] of a space group H can be done by inverting the data on the subgroups H_s of G of index [i]. For that it is first necessary to determine all subgroups $H_s < G$ of the same index and distribute them into classes of conjugate subgroups with respect to G. It is sufficient to choose a representative H_r from each class of conjugate subgroups, specified by $(\boldsymbol{P}, \boldsymbol{p})_r$, and apply $(\boldsymbol{P}, \boldsymbol{p})_r^{-1}$ to the group G in order to obtain the supergroup G_r. Further supergroups may be generated by the coset representatives of the decomposition of $N_A(H)$ relative to $(N_A(H) \cap N_A(G))$. In order to obtain all supergroups of a given space group type and index it is sufficient to apply the procedure to one representative of each class of conjugate subgroups $H_s < G$ of index [i].

Input Information of MINSUP

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

• The type of supergroup, it can be chosen from a table (returned by the program) 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.

• It is necessary to select the type of the normalizers of the group and the supergroup. By default the Euclidean normalizers of general cell metrics are used as listed in Tables 15.2.1.3 and 15.2.1.4 of *IT*A. The affine normalizers of the space groups (except triclinic and monoclinic) are also accessible.

Input Information of SUPERGROUPS

• The *IT*A numbers of the space groups G and H, and their index.

• The type of the normalizers of the group and the supergroup. As in the case of MINSUP, the spacegroup normalizers used by default are the Euclidean normalizers. Also, there is a possibility for the user to use the affine normalizers given in *IT*A or to provide a specific one.

Output Information of MINSUP and SUPERGROUPS

1. The transformation matrix $(\boldsymbol{P}, \boldsymbol{p})$ that relates the default basis of the supergroup with that of the subgroup.

2. One representative from each coset in the decomposition of the supergroup G with respect to the group H.

3. The full cosets of the decomposition $G : H$. The elements of G are listed with respect to the default basis of the subgroup H.

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 'purely' group-theoretical problem: Given a group–subgroup pair of space groups, $G > H$, determine all supergroups G of H, isomorphic to 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. As a consequence, in some particular cases when the supergroups and the groups belong to different crystal systems, it may happen that the determined supergroups are not space groups but just affine groups isomorphic to space groups (*cf.* [18]).

The number of supergroups of a space group H of a finite index is not always finite. This is the case of a space group H whose normalizer $N(H)$ contains continuous translations in one, two or three independent directions (*cf.* *IT*A, Part 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 are up to three parameters r, s and t in the transformation matrix and in the translational part of the coset representatives. The different values of the parameters corresponds to different supergroups of the same space-group type.

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

Consider two group–subgroup related space groups $G > H$. Atoms which are symmetrically equivalent under G, *i.e.* belong to the same orbit of G, may become non-equivalent under 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 $G > H$ have been treated in detail by Wondratschek [28]. Part 3 of *IT*A1 contains the tables of the Wyckoff-position splittings for all space groups and their maximal subgroups. However, for certain applications it is more comfortable to have the appropriate computer tools for the calculations of the Wyckoff-position splittings for $G > H$: for example, when H is not a maximal subgroup of G, or when the space groups $G > H$ are related by transformation matrices different from those listed in the tables of *IT*A1. The program WYCKSPLIT [20] calculates

the Wyckoff-position splittings for any group–subgroup pair. In addition, the program provides further information on Wyckoff-position splittings that is not listed in *IT*A1, namely, the relations between the representatives of the orbit of G and the corresponding representatives of the suborbits of H.

3.3.1. The program WYCKSPLIT

The program WYCKSPLIT calculates the splitting of the Wyckoff positions for a group–subgroup pair $G > H$, given the corresponding transformation relating the coordinate systems of G and H. The additional data on the explicit correspondence between the representatives of the orbit of G and the corresponding representatives of the suborbits of H are calculated by comparing the values of the fixed parameters and the variable parameter relations in both sets.

Input Information

• The specification of the space groups G and H by their *IT*A numbers.

• The transformation matrix–column pair ($\boldsymbol{P}$, $\boldsymbol{p}$) that relates the basis of G to that of H. The user can input a specific transformation or can be linked to the *IT*A1 database for the maximal subgroups of G. In the case of a non-maximal subgroup, the program SUBGROUPGRAPH provides the transformation matrix(ces) for a specified index of H in G. The transformations are checked for consistency with the default settings of G and H used by the program.

• The Wyckoff positions W_G to be split can be selected from a list. In addition, it is possible to calculate the splitting of any orbit specified by the coordinate triplet of one of its points.

Output Information

1. The splittings of the selected Wyckoff positions W_G into Wyckoff positions W_H^l of the subgroup, specified by their multiplicities and Wyckoff letters.

2. 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 W_G are referred to the bases of the group and of the subgroup.

4. REPRESENTATIONS OF CRYSTALLOGRAPHIC POINT GROUPS AND SPACE GROUPS

The *Bilbao Crystallographic Server* provides several programs facilitating the application of representation theory to specific problems of solid-state physics and crystallography-related fields. The computing packages support certain essential (and more involved from a mathematical point of view) steps in the related group-theoretical studies. The server offers access to the basic modules for handling space-group (REPRES) and point-group (POINT) representations, it enables the study of the correlations between irreps of group-subgroup related space groups (CORREL) and the decomposition of Kronecker direct products of space-group irreps (DIRPRO). In the following, we explain the necessary input data and provide details on the output results of the basic programs REPRES and POINT. For a presentation of the rest of the programs treating representations of crystallographic groups and the group-theoretical background of the developed programs, the reader is referred to Ref. [3].

4.1. Space-group representations

There exist several reference sets of tables of space-groups irreps (see *e.g*. CDML, and the references therein). However, the available data have important drawbacks related to the lack of full space-group representations due to the limitations and/or specificity in the choice of the **k**-vectors. In addition, the used space-group settings are often not compatible with those of *IT*A. These disadvantages are overcome by the program REPRES which computes the irreps of space groups explicitly: For any space group G and a **k**-vector, the corresponding little group $G^{\mathbf{k}}$, the allowed (small) irreps of $G^{\mathbf{k}}$ and the matrices of the full-group irreps are constructed. As part of the working environment of the Bilbao Crystallographic Server, the program REPRES provides the irrep data in a format suitable for its further use as input for other programs on the server.

4.1.1. The program REPRES

REPRES calculates the irreps of space groups following a general scheme based on a normal-subgroup induction method: the irreps of a space group G are constructed starting from those of its translation subgroup T_G which is a normal subgroup of G, $T_G \lhd G$. The main steps of the procedure involve the construction of all irreps of T_G and their distribution into orbits under G, determination of the corresponding little groups and the allowed (small) irreps and finally, construction of the irreps of G by induction from the allowed irreps. The most involved step in the procedure is the determination of the allowed irreps of the little group. In the majority of books on irreps of space groups this problem is solved by applying the theory of the so-called *projective representations*. Here we have preferred another approach for the construction of the allowed irreps which is a slight modification of an induction procedure originally proposed by Zak

[30]. It is based on the fact that all space groups are *solvable groups*, *i. e.* for every space group one can construct a composition series $G \rhd H_1 \rhd H_2 \ldots \rhd T$ such that all factor groups H_i/H_{i+1} are cyclic groups of order 2 or 3.

Input Information

• Space group data: As an input the program needs the specification of the space group G which can be defined by its sequential *IT*A number. Here, as well as in the rest of programs of the *Bilbao Crystallographic Server* the default settings of the space groups are used for the calculations. The program REPRES can treat space groups in unconventional settings, once the transformation matrixcolumn pair (***P***, ***p***) to the corresponding default setting is known.

• **k**-vector data: There are two different ways to introduce the **k**-vector: either by choosing it from a table where the different symmetry types of wave vectors are listed explicitly, or by typing in the **k**-vector coefficients directly. The program accepts **k**-vector coefficients referred to different coordinate systems of the reciprocal space. For its internal calculations REPRES uses **k**-vector coefficients (k_1, k_2, k_3) referred to a basis which is dual to the default ITA settings of the space groups (called conventional k-vector coefficients). The program accepts also **k**-vector coefficients referred to a primitive basis of the reciprocal lattice as given for example, in CDML tables of space-group irreps. If a non-conventional setting for the space group is chosen (2.1.1), then the corresponding 'non-conventional' **k**-vector coefficients

$$(\mathrm{k}'_1, \mathrm{k}'_2, \mathrm{k}'_3) = (\mathrm{k}_1, \mathrm{k}_2, \mathrm{k}_3)\boldsymbol{P},$$

can be given as input data. Note that the program does not accept variables (free parameters) as coefficients of the wave vector.

Output Information

1. Information on the space group G:

• Non-translational generators of G listed as matrix-column pairs (W, w), *i.e.* in (3. 4) matrix form consisting of a (3 × 3) matrix part W and a (3 × 1)-column part w:

$$(W, w) = \begin{pmatrix} W_{11} & W_{12} & W_{13} & w_1 \\ W_{21} & W_{22} & W_{23} & w_2 \\ W_{31} & W_{32} & W_{33} & w_3 \end{pmatrix};$$

The sequence of generators follows that of *IT*A for the conventional settings of the space groups;

• List of the coset representatives (W, w) of the decomposition of G with respect to T_G (known also as *translational coset representatives* given in (3 × 4) matrix form. The numbers coincide with the sequential numbers of the general-position coordinate triplets listed in *IT*A.

2. **k**-vector data:

The program lists the input values of the **k**-vector coefficients followed by the corresponding conventional coefficients ($\mathrm{k}_1, \mathrm{k}_2, \mathrm{k}_3$). The coefficients of the arms of the wave-vector star ***k** are referred also to the basis that is dual to the default setting of the space group. The program also asignes a label to the given **k**-vector according to the classification scheme of CDML.

3. Information on the little group G^{k}:

• A set of coset representatives of G with respect to the little group G^{k};

• A set of non-translational generators and a set of translational coset representatives of G^{k} given as (3×4) matrices;

• Little-group irreps presented in a matrix form for the translational coset representatives of G^{k} in a consecutive order. The labels of the irreps follow the classification scheme of CDML. The (complex) matrix elements are specified by their moduli and phase angles in degrees [○].

4. Full-group representations:

The program lists the characters of the full-group representations for all translational coset representatives of the group G. In addition, the pairs of full-group irreps that form physically-irreducible representations are also indicated.

As an option, the program can list the full-group irreducible representations of the non-translational generators of the space group (or any element of the space group specified by the user) in a blockmatrix form: for a given representation and a generator, the program prints out the induction matrix whose non-zero entries, specified by its row and column indices, indicate a matrix block corresponding to a little-group matrix.

Example: Irreps of $P4_2/mbc$ (No. 135) for **k** = **T**(0.37, 1/2, 1/2)

The input data consists in the specification of the space group $P4_2/mbc$ by its *IT*A number, No. 135, and the data for **k**-vector coefficients, **k** = T(0.37, 1/2, 1/2).

The discussion of the output follows the order of the results as they appear in the output file.

1. *Space-group information* block:

(a) The generators of $P4_2/mbc$ (with the exception of the generating translations) are listed in the same sequence as they appear in *IT*A: (1, o), (2_z, o), (4_z, τ_1), (2_y, τ_2) ($\bar{1}$, o), with o = (0, 0, 0), τ_1 = (0, 0, 1/2) and τ_2 = (1/2, 1/2, 0)[2].

[2] To make the description more compact we use a symbolic notation for the space-group elements.

(b) Decomposition of $P4_2/mbc$ relative to its translation subgroup with coset representatives as given in *IT*A: $(1, o)$, $(2_z, o)$, $(4_z, \tau_1)$, $(4^3_z, \tau_1)$, $(2_x, \tau_2)$, $(2_y, \tau_2)$, $(2_{xx}, \tau_1+\tau_2)$, $(2_{x\bar{x}}, \tau_1+\tau_2)$, $(\bar{1}, o)$, (m_z, o), $(\bar{4}_z, \tau_1)$, $(4^3_z, \tau_1)$, (m_x, τ_2), (m_y, τ_2), $(m_{xx}, \tau_1+\tau_2)$ $(m_{x\bar{x}}, \tau_1+\tau_2)$.

2. **k**-*vector information* block:

(a) The input **k**-vector coefficients **T**(0.37, 1/2, 1/2) followed by the corresponding conventional coefficients. (In all space groups with primitive lattices, the **k**-vector coefficients, referred to a primitive basis of the reciprocal space (CDML), coincide with the conventional k-vector coefficients.)

(b) The **k**-vector star: *T = {(0.37, 1/2, 1/2), (0.63, 1/2, 1/2), (1/2, 0.37, 1/2), (1/2, 0.63, 1/2)}.

(c) The little group $G^T = P2_1am$ is specified by the coset representatives of its decomposition with respect to the translation subgroup: $(1, o)$, $(2_x, \tau_2)$, (m_z, o), (m_y, τ_2). The little co-group $\bar{G}^T = \{1, 2_x, m_y, m_z\}$ is isomorphic to the point group $2_z mm$.

(d) The coset representatives of the decomposition of $P4_2/mbc$ relative to $P2_1am$ are as follows: $\{(1, o), (2_z, o), (4_z, \tau_1)$, and $(4^3_z, \tau_1)\}$.

3. *Allowed irreps* of G^T

As the little group G^T is non-symmorphic and the k vector is on the surface of the Brillouin zone, it is not possible to derive directly the allowed irreps of $P2_1am$ from the point-group irreps of the little co-group $2mm$. The program determines the allowed irreps following the composition series for the little group $P2_1am$: $P2_1am \rhd Pm \rhd T$.

The little group of the **k**-vector has 4 allowed irreps:

$P2_1am$	$(1, o)$	$(2_x, \tau_2)$	(m_x, o)	(m_x, τ_2)
$D^{T,1}$	1	ε_1	1	ε_1
$D^{T,2}$	1	ε_1	$\bar{1}$	ε_2
$D^{T,3}$	1	ε_2	$\bar{1}$	ε_1
$D^{T,4}$	1	ε_2	1	ε_2

$\varepsilon_1 = exp(i113.4)$ and $\varepsilon_2 = exp(i293.4)$

4. *Full-group irreps*

The (complex) characters of the full-group irreps for all translational coset representatives of $P4_2/mbc$ are represented by by their moduli and phase angles in degrees [○]. The physicallyirreducible representations are formed by the pairs $\{D^{*T,1}, D^{*T,4}\}$ and $\{D^{*T,2}, D^{*T,3}\}$.

The matrices of the full-group irreps for the non-translation generators are presented in a blockmatrix form. The program lists separately the induction matrix $M(W, w)$ and the corresponding blocks of the little-group representation matrices specified by the row-column indices of the nonzero entries of M (W, w). For example, the matrix of the full-group irrep for the generator $(\bar{1}, o)$ of $P4_2/mbc$ (No. 5 in the list of generators)

$$D^{*T,1}(\bar{1}, o) = \left(\begin{array}{cc|cc} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 1 \\ 0 & 0 & \bar{1} & 0 \end{array}\right)$$

is presented as a (4 × 4) induction matrix

$$M(\bar{1}, o) = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix},$$

with the following (1 × 1) blocks:

Block (1, 2) = (1.000, 0.0);
Block (2, 1) = (1.000, 0.0);
Block (3, 4) = (1.000, 180.0);
Block (4, 3) = (1.000, 180.0).

4.2. Point group representations

The information about the 32 (non-magnetic) crystallographic point groups plays a fundamental role in many applications of crystallography. In the literature, there exists a lot of information about crystallographic point groups and their representations. Some complete tables are given in Koster et al. [19], Bradley & Cracknell [7], Altmann & Herzig [1] (and the references therein). In our case, a selection of these data have been recalculated and is now available online via the *Bilbao Crystallographic Server*. The point-group databases are part of the core shell of the server. They provide essential information for a point-group analysis in applications related to crystallographic, solid-state or phase transitions problems. The information about the irreps of the 32 point groups is obtained from the program REPRES for the particular case of **k** = Γ(0, 0, 0). The generated point-group data have been stored as an XML database of the server.

4.2.1. The program POINT

The program POINT displays a set of tables for each of the 32 crystallographic point groups which are specified by their international (Hermann-Mauguin) and Schoenflies symbols:

1. Character table. The character table provides the characters of the ordinary irreps of the chosen point group. The irreps are labelled in the notation of Mulliken [24] and by the Γ labels introduced by Bethe [6], see also Koster et al. [19]. The matrices

of the degenerate irreps as calculated by REPRES are also accessible. The number of point-group elements in a conjugacy class is indicated by the listed multiplicity. In addition, the transformation properties of the cartesian tensors of rank 1 (vectors and axial vectors) and 2 are displayed. (The tensor of rank 0 belongs always to the totally symmetric irrep and is not listed explicitly). Cartesian tensors that transform according to two- or three-dimensional irreps are joined by brackets.

2. Subgroup table. The point-group types of the subgroups of a point group are listed with the corresponding indices with respect to the initial point group.

3. Irrep multiplication table. The table shows the decomposition into irreducible constituents of the Kronecker (direct) product of any pair of point-group irreps.

4. Tensor representations. A physical property can be represented by a tensor which transforms, in general, according to a reducible representation. Any reducible representation can be decomposed into irreducible constituents applying the so-called reduction ("magic") formula:

$$\Gamma \sim \bigoplus_i n_i \Gamma_i, \text{ where } n_i = \frac{1}{|\overline{G}|} \sum_{\mathrm{g}} \chi(\mathrm{g}) \chi_i^*(\mathrm{g}).$$

Here, Γ represents a reducible representation expressed in terms of its irreps Γ_i. The multiplicity of the irrep is given by n_i, $|\overline{G}|$ is the order of the point group and $\chi(\mathrm{g})$ and $\chi_i(\mathrm{g})$ are the corresponding characters of the reducible representation Γ and the irrep Γ_i.

The tensor-representation tables one finds the decompositions into irreducible constituents of representations related to some important tensors (and their powers), such as the vector V (polar) or the pseudovector A (axial), their symmetrized $[V^2]$ or antisymmetrized squares, *etc*.

5. Selection rules for fundamental transitions. The table displays the selection rules for infrared and Raman vibrational (phonon) transitions. The data in the first row of each table (specified by the trivial irrep label) corresponds to the usual infrared and Raman selection rules.

6. Subduction from the rotation group irreps. Given a representation of the rotation group of dimension $2l+1$, $l = 0,\ldots,9$, the table lists the point-group irreps which appear in its subduction to the chosen point group.

5. CONCLUSIONS

The *Bilbao Crystallographic Server* site provides a free online interface for different crystallographic databases and programs at www.cryst.ehu.es. The working enviroment is divided into several shells according to different topics, from simple retrieval tools for access to crystallographic data to more sophisticated solid-state applications.The programs available on the server do not need a local installation the only requirement is an Internet connection and a web browser. The programs on the *Bilbao Crystallographyc Server* have user-friendly interfaces with links to documentation an online 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 dato to other. In that way the server has turned into a workin environment with the appropiate tools for treating problems of theoretical crystallography, solid-state physics and crystal chemistry.

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КРИСТАЛОГРАФИЯ ОНЛАЙН: БИЛБАО КРИСТАЛОГРАФСКИ СЪРВЪР

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(Резюме)

Билбао Кристалографски Сървър е уебсайт с кристалографски база данни и програми, достъпни онлайн (www.cryst.ehu.es). В продължение на повече от 10 години сървърът предоставя кристалографска информация, като предлаганите данни и програми постоянно се обновяват и разширяват. Програмите на сървъра не се нуждаят от локално инсталиране и могат да бъдат използвани безплатно. Билбао Кристалографски Сървър предоставя свободен достъп до информация от общ характер свързана с кристалографските групи на симетрия (генератори, общи и специални Wyckoff позиции, зони на Brillouin и т.н.). Освен приложенията за директно четене на съхраняваните данни, сървърът разполага с програми за анализ на връзките група–подгрупа за пространствените групи, техните представяния и т.н. Има също така програмни продукти за изучаване на специфични проблеми от физиката на твърдото тяло, структурна химия и кристалография.