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1.7. The Bilbao Crystallographic Server

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1.7.1. Introduction

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

The server is built on a core of databases and contains different shells. The set of databases includes data from the 5th edition of *International Tables for Crystallography* Volume A, *Space-Group Symmetry* (2005) (hereafter referred to as *IT* A) and the data for maximal subgroups of space groups as listed in Part 2 of this volume (hereafter referred to as *IT* A1). Access is also provided to the crystallographic data for the subperiodic layer and rod groups [*International Tables for Crystallography*, Volume E, *Subperiodic Groups* (2002)] 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 wavevectors for space groups are also available.

Communication with the databases is achieved by simple retrieval tools. They allow access to the information on space groups or subperiodic groups in different types of formats: HTML, text ASCII or XML. The next shell includes programs related to group–subgroup relations of space groups. 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. There follows a shell with programs on representation theory of space groups and point groups and further useful symmetry information. Parallel to the crystallographic software, a shell with programs facilitating the study of specific problems related to solid-state physics, structural chemistry and crystallography has also been developed.

The server has been operating since 1998, and new programs and applications are being added (Kroumova, Perez-Mato, Aroyo *et al.*, 1998; Aroyo, Perez-Mato *et al.*, 2006; Aroyo, Kirov *et al.*, 2006). The aim of the present chapter is to report on the different databases and programs of the server related to the subject of this volume. Parts of these databases and programs have already been described in Aroyo, Perez-Mato *et al.* (2006), and here we follow closely that presentation. The chapter is completed by the description of the new developments up to 2007.

The relevant databases and retrieval tools that access the stored symmetry information are presented in Section 1.7.2. The discussion of the accompanying applications is focused on the crystallographic computing programs related to group–subgroup and group–supergroup relations between space groups (Section 1.7.3). The program for the analysis of the relations of the Wyckoff positions for a group–subgroup pair of space groups is presented in Section 1.7.4. The underlying group-theoretical background of the programs is briefly explained and details of the necessary input data and the output are given. The use of the programs is demonstrated by illustrative examples.

1.7.2. Databases and retrieval tools

The databases form the core of the Bilbao Crystallographic Server and the information stored in them is used by all computer programs available on the server. The following description is restricted to the databases related to the symmetry relations between space groups; these are the databases that include space-group data from *IT* A and subgroup data from *IT* A1.

1.7.2.1. Space-group data

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 at $\overline{1}$) for the centrosymmetric groups listed with respect to two origins in *IT* A.

The space-group database includes the following symmetry information:

(i) The generators and the representatives of the general position of each space group specified by its *IT* A number and Hermann–Mauguin symbol;
(ii) The special Wyckoff positions including the Wyckoff letter, Wyckoff multiplicity, the site-symmetry group and the set of coset representatives, as given in *IT* A;
(iii) The reflection conditions including the general and special conditions;
(iv) The affine and Euclidean normalizers of the space groups (*cf. IT* A, Part 15). They are described by sets of additional symmetry operations that generate the normalizers successively from the space groups. The database includes the additional generators of the Euclidean normalizers for the general-cell metrics as listed in Tables 15.2.1.3 and 15.2.1.4 of *IT* A. These Euclidean normalizers are also affine normalizers for all cubic, hexagonal, trigonal, tetragonal and part of the orthorhombic space-group types. For the rest of the orthorhombic space groups, the type of the affine normalizer coincides with the highest-symmetry Euclidean normalizer of that space group and the corresponding additional generators form part of the database (*cf.* Table 15.2.1.3 of *IT* A). The affine normalizers of triclinic and monoclinic groups are not isomorphic to groups of motions and they are not included in the normalizer database of the Bilbao Crystallographic Server.
(v) The assignment of Wyckoff positions to Wyckoff sets as found in Table 14.2.3.2 of *IT* A.

The data from the databases can be accessed using the simple retrieval tools, which use as input the number of the space group (*IT* A numbers). It is also possible to select the group from a table of *IT* A numbers and Hermann–Mauguin symbols. The output of the program *GENPOS* contains a list of 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. A list of the Wyckoff positions for a given space group in different settings can be obtained using the program *WYCKPOS*. The Wyckoff-position representatives for the nonstandard settings of the space groups are specified by the transformed coordinates of the representatives of the corresponding default settings. The assignments of the Wyckoff positions to Wyckoff sets are retrieved by the program *WYCKSETS*. This program also lists a set of 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 programs *NORMALIZER* and *HKLCOND* give access to the data for normalizers and reflection conditions.

1.7.2.2. Database on maximal subgroups

1.7.2.2.1. Maximal subgroups of indices 2, 3 and 4 of the space groups

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*. Each subgroup $\mathcal{H}$ is specified by its *IT* A number, the index in the group $\mathcal{G}$ and the transformation matrix–column pair $(\boldsymbol{P}, \boldsymbol{p})$ that relates the bases of $\mathcal{H}$ and $\mathcal{G}$:

$$(\mathbf{a}', \mathbf{b}', \mathbf{c}')_{\mathcal{H}} = (\mathbf{a}, \mathbf{b}, \mathbf{c})_{\mathcal{G}}\boldsymbol{P}. \qquad (1.7.2.1)$$

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 $\mathcal{G}$.

It is important to note that, in contrast to the data listed in *IT* A1, the matrix–column pairs $(\boldsymbol{P}, \boldsymbol{p})$ used by the programs of the server transform the *standard* basis $(\mathbf{a}, \mathbf{b}, \mathbf{c})_{\mathcal{G}}$ of $\mathcal{G}$ to the *standard* basis of $\mathcal{H}$ (see Section 2.1.2.5 for the special rules for the settings of the subgroups used in *IT* A1). The different maximal subgroups are distributed in classes of conjugate subgroups. 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 $(\boldsymbol{P}, \boldsymbol{p})^{-1}$ to the coordinate system of $\mathcal{G}$. In addition, one can obtain the splittings of all Wyckoff positions of $\mathcal{G}$ to those of $\mathcal{H}$.

1.7.2.2.2. Maximal isomorphic subgroups

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 as members of series under the heading 'Series of maximal isomorphic subgroups'. In addition, the isomorphic subgroups of indices 2, 3 and 4 are listed individually. The program *SERIES* provides access to the database of maximal isomorphic subgroups on 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 maximum index is 125. The format and content of the subgroup data are similar to those of the *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 generated online and do not form part of the (static) database of isomorphic subgroups.]

1.7.3. Group–subgroup and group–supergroup relations between space groups

1.7.3.1. Subgroups of space groups

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 $\mathcal{H}$. We have developed two basic tools for the analysis of the group–subgroup relations between space groups: *SUBGROUPGRAPH* (Ivantchev *et al.*, 2000) and *HERMANN* (Capillas, 2006). Given the space-group types $\mathcal{G}$ and $\mathcal{H}$ and an index [i], both programs determine all different subgroups $\mathcal{H}_j$ of $\mathcal{G}$ with the given index and their distribution into classes of conjugate subgroups with respect to $\mathcal{G}$. Owing 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*.

1.7.3.1.1. The program SUBGROUPGRAPH

This 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 nodes corresponding to the 230 space-group types. If two nodes 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 standard 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 node and $\mathcal{H}$ as the bottom node, see Example 1.7.3.1.1 at the end of this section. 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 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 nodes in the general $\mathcal{G} > \mathcal{H}$ graph may be further reduced if the index of $\mathcal{H}$ in $\mathcal{G}$ is specified. The subgraph obtained is again of the contracted type.

The comparison of complete graphs and contracted graphs shows that the use of contracted graphs for the analysis of specific group–subgroup relations $\mathcal{G} > \mathcal{H}_j$ can be very misleading (see Example 1.7.3.1.1, Fig. 1.7.3.2 and Fig. 1.7.3.3). The complete graphs produced by *SUBGROUPGRAPH* are equal for subgroups of a conjugacy class; the different orientations and/