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

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