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SUBGROUPGRAPH: a computer program for analysis of group–subgroup relations between space groups

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1. The crystallographic problem

Group–subgroup relations between two space groups, $G > H$, are of essential importance for phase-transition problems: for determination of the relation between the low- and high-symmetry structures, domain structure analysis, displacement-mode analysis, *etc*. The available subgroup data in the *International Tables for Crystallography*, Vol. *A* (1995), are not sufficient for a detailed treatment of $G > H$ relations. The necessary data will be available in the forthcoming Vol. *A*1 of the *International Tables for Crystallography* (2001). The program *SUBGROUPGRAPH* uses a preliminary CIF version of the Vol. *A*1 database (Wondratchek *et al.*, 1996).

The main aim of *SUBGROUPGRAPH* is a detailed study of a group–subgroup relation between two space groups, including the construction of chains of maximal subgroups for $G > H$ for a specified/non-specified index $i = |G{:}H|$ (the so-called *G–H* graph), the determination of the number of different $H_k < G$, $H_k \cong H$, and their distribution into classes of conjugate subgroups relative to *G*, *etc*.

2. Method of solution

As a first step, the program inverts the Vol. *A*1 database into a general graph with 230 vertices (points) corresponding to the 230 space groups: an edge (line) connects two vertices if there exists a maximal group–subgroup relation between the corresponding groups. The isomorphic subgroups (restricted to those of indices 2, 3 and 4) are represented by loops. The *G–H* graph is a subgraph of the general one whose top and bottom vertices are the groups *G* and *H*. Once the index *i* is specified, *SUBGROUPGRAPH* determines all possible chains of maximal subgroups relating *G* and *H*: (i) by factorization of *i* into factors 2, 3 and 4 (possible indices of non-isomorphic maximal subgroups and the considered isomorphic ones); (ii) using the *G–H* graph and the corresponding Vol. *A*1 data, the program specifies the different $G > H_k$ chains by the transformation matrices relating the group and subgroup bases. The identification of the different (relative to *G*) subgroups H_k and their distribution into conjugacy classes with respect to *G* is performed directly, by analysing the subgroups H_k and their interrelations in the *G* basis. The results obtained using this method can be compared with those returned from the normalizer procedure described by Koch (1984).

3. Software environment

SUBGROUPGRAPH runs under any Unix or Unix-like operating system (Digital Unix, HP-UX, Sun, BSD, Linux, *etc*.). *SUBGROUPGRAPH* is written in C and Perl. Only standard library functions are used. No overlay structure has been applied. The *daVinci* system (Frohlich & Werner, 1996) is used for the representation of group–subgroup graphs.

4. Hardware environment

The program runs on any computer with the Unix operating system (Intel, Alpha, Sparc, Mips, *etc*.). The amount of memory used depends of the complexity of the *G–H* graph. The program requires the *International Tables for Crystallography*, Vol. *A*1, in CIF format (4000 kbyte of disk space). However, the program can be used *via* the Internet (from any Unix, VMS, Macintosh, DOS, Windows, *etc*., platform), thus not necessitating local installation.

5. Program specifications

Input: groups *G* and *H*, and the index of *H* in *G*. The data for *G* and *H* follow the conventions in the *International Tables for Crystallography*, Vols. *A* and *A*1, with the following restrictions: unique axis *b* setting for the monoclinic groups, hexagonal axes setting for the rhombohedral groups, and origin 2 choice for the centrosymmetric groups listed with respect to two origins in the *International Tables for Crystallography*, Vol. *A*.

Output: (i) a general $G > H$ graph where the index *i* of *H* in *G* is not specified; (ii) all possible chains of maximal subgroups connecting *G* and *H* for a specified value of *i* (the corresponding transformation matrices relating the bases of the group and subgroup are also listed); (iii) the identification of the different (relative to *G*) subgroups H_k and their distribution into classes of conjugate subgroups with respect to *G*; (iv) a $G > H$ graph of chains of maximal subgroups for the specified index of the subgroup where all different subgroups H_k are indicated.

6. Documentation and availability

An on-line description of the input and the output of the program, as well as a description of the method, is available at http://www.cryst.ehu.es/sg_graph_doc.html. The program forms part of the Bilbao Crystallographic Server, http://www.cryst.ehu.es (Kroumova *et al.*, 1998, 1999), and uses the databases and the results from other programs available on this server. *SUBGROUPGRAPH* can be used *via* the Internet from any computer with a Web browser. The URL of the program is http://www.cryst.ehu.es/subgroupgraph.html.

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