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computer program abstracts

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SUPERGROUPS – a computer program for the determination of the supergroups of the space groups

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1. The crystallographic problem

The problem of the determination of the supergroups of a given space group is of rather general interest. It is useful in phase-transition problems, in the search for overlooked symmetries in a crystal structure determination, or in the detection of pseudosymmetries as a tool for predicting higher-temperature phase transitions (Igartua *et al.*, 1996). In all these applications, it is not sufficient to know the space-group types of the supergroups of a given group; rather, it is necessary to have available all the different supergroups $\mathcal{G}_j > \mathcal{H}$ 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 & Aroyo, 2001). In the *International Tables for Crystallography*, Vol. A, *Space Group Symmetry* (1983), 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, *i.e* to which minimal supergroups of $\mathcal{H}$ belong. It is rather difficult to determine all supergroups $\mathcal{G}_j > \mathcal{H}$ if only the types of the minimal supergroups are known. The program *SUPERGROUPS* solves this problem for a given finite index [*i*].

2. Method of solution

The method for the determination of the supergroups $\mathcal{G}_j$ of $\mathcal{H}$ used by *SUPERGROUPS* is based on the explicit data of maximal subgroups of space groups, which will be available in the forthcoming Vol. A1 (*Symmetry Relations Between Space Groups*) of the *International Tables for Crystallography*. The procedure involves two main steps. Given a pair of space groups $\mathcal{G} > \mathcal{H}$ and an index, the program finds different chains of minimal supergroups between $\mathcal{H}$ and $\mathcal{G}$ by inverting the subgroup data of Vol. A1 of the *International Tables for Crystallography*. The chains are distinguished by the corresponding transformation matrices that relate the bases of $\mathcal{H}$ and $\mathcal{G}$. The minimal isomorphic supergroups are restricted to those with indices 2, 3 and 4. All different supergroups $\mathcal{G}_j \cong \mathcal{G}$ of $\mathcal{H}$ are obtained in the second step of the procedure by applying the space-group normalizer procedure (Koch, 1984) for each of the chains retrieved from the *International Tables for Crystallography*, Vol. A1, database.

For example, suppose the minimal *P*23 supergroups of a space group *P*222 are to be determined from the corresponding data on maximal subgroups in Vol. A1 of the *International Tables for Crystallography*. There is only one maximal subgroup *P*222 of a space group *P*23 of index 3 and thus one minimal supergroup of *P*222 obtained in the first step. The application of the normalizer procedure to this supergroup gives four minimal supergroups of *P*222 belonging to the type *P*23, which are distinguished by their conventional origins with respect to the conventional setting of *P*222: 0, 0, 0; $\frac{1}{2}$, 0, 0; 0, $\frac{1}{2}$, 0; 0, 0, $\frac{1}{2}$. The supergroups $Pm\bar{3}$ of *P*222 of index 6 are obviously not minimal, as $Pm\bar{3} > P23 > P222$. Again, to the only one subgroup *P*222 of $Pm\bar{3}$ of index 6, there correspond four different supergroups $Pm\bar{3}$ of the group *P*222, because each of the supergroups *P*23 carries exactly one supergroup $Pm\bar{3}$.

3. Software and hardware environment

The package *SUPERGROUPS* runs under any Unix or Unix-like operating system (Digital Unix, HP-UX, Sun, BSD, Linux, *etc.*). It is written in C. Only standard library functions are used. Parts of the program in which data are extracted from CIF files are written in Perl. No overlay structure has been applied. The program is designed to be used without local installation from any computer with a Web browser (Unix, VMS, Macintosh, DOS, Windows, *etc.*).

4. Program specification

Input: the space groups $\mathcal{G}$ and $\mathcal{H}$, and the index [*i*]. The space-group normalizers (necessary for the second step of the procedure) used by default are the Euclidean normalizers listed in Table 15.3.2. of Vol. A of the *International Tables for Crystallography*. The user can also apply the affine normalizers listed in that table. For a translation lattice with metrics of apparent higher symmetry, the user may provide the set of additional generators for the 'augmented' Euclidean normalizer.

Output: list of all supergroups $\mathcal{G}_j$ of $\mathcal{H}$, isomorphic to $\mathcal{G}$ and of the same index. The supergroups $\mathcal{G}_j$ are referred to the basis of the subgroup $\mathcal{H}$ and are represented by the coset representatives of $\mathcal{G}_j$ relative to $\mathcal{H}$.

5. Documentation

A user manual with a description of input and output of the program is available online at http://www.cryst.ehu.es/cryst/sup_help.html.

6. Availability

The program *SUPERGROUPS* 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. The program, at http://www.cryst.ehu.es/cryst/supergroups.html, can be used from any computer with a Web browser.

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