Computer Program Abstracts

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WYCKSPLIT: a computer program for determination of the relations of Wyckoff positions for a group–subgroup pair

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The crystallographic problem: During a continuous or nearly continuous phase transition the symmetry of high- and low-symmetry phases is described by 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 nonequivalent under H (*i.e.* the orbit splits) and/or their site symmetries may be reduced. The structural relation between the group–subgroup-related phases follows from the relations of the occupied orbits and this behaviour is the same for all orbits belonging to a Wyckoff position. The aim of the program is the determination of the relations of the Wyckoff positions [known as splitting of Wyckoff positions (Wondratschek, 1993)] for a group–subgroup symmetry break $G > H$.

Method of solution: Consider a group–subgroup pair $G > H$ and a transformation matrix relating the group and subgroup bases. Given an orbit O^G of G the splitting is determined as follows: (i) *WYCKSPLIT* calculates the decomposition of O^G with respect to H, into suborbits O^G_k. This is achieved *via* the splitting of the general position of G. (ii) Each suborbit O^G_k is identified with the orbits O^H of H listed in *International Tables for Crystallography* (1995) by searching among the subgroup Wyckoff positions for orbits O^H with (*a*) the same multiplicity, (*b*) the number of free parameters equal or greater than that of the orbit O^G_k, (*c*) the same characteristic numbers. If there is more than one Wyckoff position of H satisfying these conditions, then the program compares O^G_k with particular O^H orbits obtained for specific values of the parameters of the Wyckoff positions of H. In the splitting procedure described, the orbit O^G can be specified either by the corresponding Wyckoff position of G, or by one of its representative coordinate triplets.

Software environment: *WYCKSPLIT* runs under any Unix or Unix-like operating system (Digital Unix, HP-UX, Sun, BSD, Linux *etc.*). *WYCKSPLIT* is written in C. Only standard library functions are used. No overlay structure has been applied.

Hardware environment: The program runs on any computer with a Unix operating system (Intel, Alpha, SPARC, Mips *etc.*). The executable program takes about 140 kbytes of disk space and 500 kbytes memory. However, the program can be used without local installation from any computer with a WWW browser (Unix, VMS, Macintosh, DOS, Windows *etc.*).

Program specification: Input: (i) the groups G and H specified by their sequential numbers, as listed in *International Tables for Crystallography* (1995); (ii) a transformation matrix relating the bases of the group and the subgroup; (iii) the orbits O^G are selected either from a menu with Wyckoff positions of G, or by inputting the coordinate triplet of an O^G point. *WYCKSPLIT* can treat group or subgroup data in unconventional settings, once the transformation matrices to the corresponding conventional settings are known. Output: the splitting of the selected Wyckoff positions is shown in HTML form. It can be saved as a file or printed.

Documentation: A user's manual with the description of input and output of the program is included in the package. It is available online at http://lcdx00.wm.lc.ehu.es/cryst/wpsplit.html.

Availability: The program can be used without local installation from any computer with a WWW browser *via* the Internet. The URL of the documentation and the program itself is http://lcdx00.wm.lc.ehu.es/cryst/wpsplit.html.

Keywords: space groups; Wyckoff positions; group–subgroup chains.

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Notes and News

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ICDD Crystallography Scholarship Awards

To encourage promising graduate students to pursue crystallographically oriented research, the International Centre for Diffraction Data (ICDD) has established a Crystallography Scholarship Fund. Convinced of the beneficial scientific impact of the proposed scholarships, the ICDD has solicited funds from private and industrial sectors to support this program. The ICDD has awarded 24 scholarships since 1992, five in 1998.

Applicants should be graduate students seeking degrees with major interest in crystallography. There are no restrictions on country, race, age or sex. The term of the scholarship is one year. Application for one renewal may be made by the recipient at the end of the first year. Each applicant should submit a Curriculum Vitae, listing degree(s) held and degree(s) sought, a one-page proposal describing the type of research to be partly supported by scholarship, and a supportive letter from the sponsoring professor of an accredited university or an institute of technology on institution letterhead. The scholarship stipend of $2000 is to be used to help defray tuition and laboratory fees.

The awarding of the scholarships is administered by a committee. Applications must be received by 31 October 1998. Please mail to: Secretary, International Centre for Diffraction Data, 12 Campus Boulevard, Newtown Square, PA 19073-3273, USA.