Computer Program Abstracts

The category Computer Program Abstracts provides a rapid means of communicating up-to-date information concerning both new programs or systems and significant updates to existing ones. Following normal submission, a Computer Program Abstract will be reviewed by one or two members of the IUCr Commission on Crystallographic Computing. It should not exceed 500 words in length and should use the standard format given on page 189 of the June 1985 issue of the Journal [J. Appl. Cryst. (1985), 18, 189–190].

KAREP – a program for calculating irreducible space-group representations. By E. HOVE-STREYDT, *Siemens AG, Abteilung AUT V371, Postfach 211262, 7500 Karlsruhe 21, Germany,* M. AROYO, *Faculty of Physics, Blvd A. Ivanov 5, Sofia 1126, Bulgaria,* and S. SATTLER and H. WONDRAT-SCHEK, *Institut für Kristallographie, Kaiserstrasse 12, 7500 Karlsruhe 1, Germany*

The crystallographic problem: Group-theoretical methods are used in the investigation of problems such as phase transitions in crystals. A detailed knowledge of the irreducible space-group representations for certain points in reciprocal space is advantageous for such studies. Existing sets of tables have severe drawbacks such as the lack of full-matrix representations, limitations restricting the choice of the k vector to the representation domain and often the conventions used are not compatible with those of *International Tables for Crystallography* (1989). These disadvantages have been overcome by the present program *KAREP*. To aid group-theoretical analysis of crystal vibrations, computer programs for calculating irreducible representations of space groups were published in the seventies (Worlton & Warren, 1972; Neto, 1975). Later, software packages were developed that contained such programs (Davies & Dirl, 1989; Junming, Zhan & Bailin, 1990). Our goal in developing *KAREP* was a fast and flexible computer program running on a PC. It can be used on its own or as part of a program system.

Method of solution: *KAREP* calculates the irreducible representations explicitly for any space group. The program determines the little group for the k vector and obtains the allowed irreducible representations of the little group by Zak's (1960) induction procedure starting from the allowed irreducible representations of P1. In the final step the program chooses a convenient set of coset representatives of the space group with respect to the little group. It then calculates the induction matrices for these and thereby the full-matrix representation of the space group. The program thus performs all necessary crystallographic and group-theoretical calculations.

Software environment: *KAREP* is written in Fortran77. Only standard options and no overlay structure have been applied. Apart from the standard intrinsic Fortran functions and the subroutines included, no other libraries are used. The program needs for execution a small ASCII data file containing the matrices of the space-group generators.

Hardware environment: The program runs under MS-DOS 3.20 and higher on AT-compatible PCs. The executable program takes up 120 kbyte of disk space and during execution it needs 445 kbyte of memory. The program also runs on VAX and MicroVAX computers under VMS. Output is screen-oriented, up to 80 columns wide, and is simultaneously written into a file.

Program specifications: Calculations can be made for any space group. Input: (i) Space-group number for standard settings (origin choice 1; monoclinic: unique axis *b*). For unconventional settings, possibilities and restrictions are explained in the manual. (ii) The k vector, either with its coefficients referred to a primitive basis of the reciprocal lattice or specified by 'adjusted' coefficients, based on *International Tables for Crystallography* (1989) and defined in the manual. The coefficients are not restricted to any representation domain.

The program is to a large extent interactive; output can be limited to the essential minimum. By changing the translational parts of symmetry operations, representation matrices can be calculated for any element of the space group. The program can be rerun for different k vectors. Numerical input is in free format and Y/N questions have default answers to facilitate operation of the program.

Documentation: A description of the mathematical background of the various procedures used, as well as a user's manual with the description of the input and output (illustrated with an example) will be sent with the program.

Acknowledgments: The authors are grateful to Drs H.-P. Rehm and W. Trinks for their valuable help in programming and useful discussions.

Availability: Copies of *KAREP* can be obtained free of charge for non-profit-making organizations by sending a request with an MS-DOS formatted floppy disk to the first author. The files consist of Fortran77 source code, a PC-executable version (without a coprocessor) and programs to install the input files for the generators of all space groups in the standard setting.

Keywords: Irreducible representation, space-group representation, little group, induction, Zak's procedure.

References

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Crystallographers

This section is intended to be a series of short paragraphs dealing with the activities of crystallographers such as their changes of position, promotions, assumption of significant new duties, honours, etc. Items for inclusion, subject to the approval of the Editorial Board, should be sent to the Executive Secretary of the International Union of Crystallography (J. N. King, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England).

Dr **D. Louër**, Laboratoire de Cristallochimie, Université de Rennes I, France, will be the recipient of the 1992 Hanawalt Award of the International Centre for Diffraction Data.

Professor **M. M. Woolfson**, Department of Physics, University of York, England, has been awarded the 1992 Gregori Aminoff Gold Medal and Prize. The award, which recognized his many outstanding contributions to crystallography, in particular relating to the solution of the phase problem, was presented to Professor Woolfson at the Royal Swedish Academy of Sciences meeting on 20 May 1992.