A NEW VERSION OF THE PROGRAM FOR THE GENERATION OF SYMMETRY-ADAPTED FUNCTIONS FOR MOLECULAR CALCULATIONS

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A few hundred changes in the original code written in ICL 4-72 FORTRAN have been made. A new version can be compiled without any difficulties by standard FORTRAN 77 compilers.

NEW VERSION SUMMARY

Title of version: SYMMET version 2

Catalogue number: ABRA

Program obtainable from: CPC Program Library, Queen's University, Belfast, N. Ireland (see application form in this issue)

Reference to original program: catalogue number: AAPD; *title*: SYMMET; *ref. in CPC*: 24 (1981) 135

Author of original program: L. Skála

Programming language used: FORTRAN 77

Peripherals used: line printer

No. of lines in combined program and test deck: 1279

Keywords: electronic structure, molecule, symmetry-adapted function, point group, irreducible representation

Nature of physical problem
The group theory is used for the classification of the electron states of molecules and the transformation of the matrix eigenvalue problem to a quasidiagonal form. If the p-basis on any atom is used, the group analysis of the vibrational problems can also be made.

Method of solution
Symmetry-adapted linear combinations of the basis functions and other information are obtained by means of the symmetrizing operators.

Reason for the new version
Incompatibility with standard FORTRAN 77 compilers.

Restrictions on the complexity of the problem
All the most important point groups are included. There is no restriction on the number of the basis functions. The basis functions can be of s-, p- and d-type.

LONG WRITE-UP

The original program SYMMET has been modified in such a way that in can be compiled without any difficulties with standard FORTRAN 77 compilers (tests were done with seven different compilers including some compilers on personal computers). All LOGICAL * 1 declarations were changed to LOGICAL. Similarly, all INTEGER * 4 declarations were replaced by INTEGER. The changes do not effect the test run output.