for those space groups for which they occur, by use of a look-up table indexed by the reflection type and the coincidence-group number. The latter, which is derived from the space-group number, defines the appropriate generating vectors for the indices of the coincident non-equivalent reflections.

The final set of reflections is output as a list of $h, k, l$ spacing, scattering angle or flight time, and multiplicity. In addition to a line-printer listing, the reflection set can be output optionally on cards or filed as a data set in a suitable form for direct input to the Rietveld profile-analysis program. Since the generation procedure and the symmetry conditions are derived from the space-group number for any conventional space-group setting the input specification is extremely simple and the program is very convenient to use. The additional facility for generating specified types of reflections only has also proved extremely useful in providing preliminary information for single-crystal studies.

This program has been comprehensively tested and has been used successfully by people in a number of other laboratories. Full details of the program, which was written in Fortran IV for use on the Harwell IBM 370/168 computer, are given elsewhere (Cooper, Rouse & Sayers, 1977).

References


A computer program for the determination of cavity shapes and dimensions in crystal structures.

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A computer program for three-dimensional location of cavities in crystal structures and packing-density checks is presented.

Crystal structure resolution often requires the location of cavities in order to place certain molecules or atoms. In small-dimension structures, such as minerals generally are, this happens, for instance, with water molecules whose amount present is sometimes not accurately known from chemical analysis. An example occurred with naujakasite (Basso, Dal Negro, Della Guista & Ungaretti, 1975): according to the thermogravimetric analysis, this sheet silicate had 2-60% of $\text{H}_2\text{O}^-$. In the early stages of the structure solution, this program quickly excluded the presence of any cavity suitable for a water molecule.

The program, written in Fortran IV, has been debugged and tested on a CII 10070 computer (32 bits per word); core capacity ca 15 K words. Input data are: cell parameters, symmetry information and atomic coordinates in the same format required by ORFLS (Busing, Martin & Levy, 1962). Starting and finishing values on the $x$, $y$ and $z$ axes and the scan intervals are chosen by the user.

The program computes the distances from the points inside the required volume to all the atoms present in it and to those distant from its faces by an amount chosen by the user.

The printout looks like common three-dimensional Fourier analyses; in each point the minimum distance from the nearest atom is printed, allowing a survey of the shape and dimensions of channels and holes.

Each output page containing distances is followed by another containing the order number of the atoms to which each distance refers.

This three-dimensional mapping of distances may be a helpful point-by-point check of packing density.

The program is available upon request from the authors.

References