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Product Information

A NEW VERSION R-SAPI-88

A new version of the program system SAPI [1] has been released. In comparison with the old version, it possesses the following additional features:

1. Optimization has been made for the automatic solution of structures having pseudo-translational symmetry, such as superstructures. Three known and two unknown structures with pseudo-translational symmetry have been used to test the program. All of them can be solved starting from a default run of SAPI-88.

2. Automatic Patterson analysis has been included, which can be used to solve heavy-atom-containing structures. The heavy atoms are located by an automatic Harker-analysis, while the light atoms by searching for the non-Harker peaks. Combination of automatic Patterson analysis and direct methods is also possible.

3. The maximum number of reflections accepted for the direct method phasing has been extended to 1000 in the new version. This is necessary for solving certain complex structures.

4. A sophisticated menu-drive is provided for use with VAX computers.

5. The new version can easily be combined, without affecting any of its own features, with the structure-analysis package TEXSAN of the Molecular Structure Corporation.

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[1] Fan Hai-fu, Rigaku Journal 3 (1) 25-30 (1986).

(The Text of the R-SAPI-85 is as follows.)

R-SAPI-85

A COMPUTER PROGRAM FOR AUTOMATIC SOLUTION OF CRYSTAL STRUCTURES FROM X-RAY DIFFRACTION DATA

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R-SAPI-85 is a Rigaku version of SAPI-85 for use with a micro VAX computer. The name SAPI is an abbreviation of "Structure Analysis Programs with Intelligent control", it may also so be read inversely as "Institute of Physics, Academia Sinica".

SAPI-85 is based on MULTAN-80 [1] and differs from which by following:

1. The program can automatically handle diffraction data of structures having pseudo-translational symmetry and lead directly to a correct solution in favourable cases.

2. The program can recognize pseudo-centrosymmetric solutions when dealing with non-centrosymmetric structures. In addition, the program can break the enantiomorphous ambiguity given a group of atoms, each of which comes from either of the enantiomorphs.

3. Instead of the phase permutation of MULTAN-80, random starting phases are assigned to all but the origin and enantiomorph fixing reflections. A speed-up scheme is optional to use the early figure of merit with floatable cutoff value in order to save computing time.

4. The program possesses the ability of intelligent control on the path of phase development according to the complexity of the structure and the early stage result during the phase development.

5. The programs EXFFT and SEARCH of MULTAN-80 have been extended to include the calculation and peak search for Patterson and minimum functions. This enables the effective combination of Patterson and direct methods.

6. The program can output density maps, sections or composite sections, as "half-tone graphs" on a conventional lineprinter. The size and contrast of the map output can be controlled automatically or manually.

7. The program for the interpretation of space group symbols written by Burzlaff and Hountas [2] has been modified and included.

For the theoretical background on the treatment of pseudo symmetry, the reader is referred to Fan Hai-fu & Zheng Qi-tai [3], Fan Hai-fu [4] and the references therein. For the detail of the random starting procedure used in this program system, see Yao Jia-xing [5].

The complete system of SAPI-85 is made up of the following:

"PREPAR": perform the preliminary processing of F(obs) data for later use.

"PHASE": solve the phase problem using direct methods.

"EXFFT": fast Fourier transform program.

"SEARCH": interpret the output of "EXFFT".

"MAP": output density maps.

Included in the program "PREPAR", there is a subroutine "AUTOGP". It scans the E values and searchs for pseudo-systematic extinction. Once this is found, reflections will be grouped automatically according to the pseudo-systematic-extinction rule and the program will print out message like this:

PSEUDO-TRANSLATIONAL SYMMETRY HAS BEEN FOUND BY THE PROGRAM ***NORMALIZATION IS TO BE RESTARTED*** REFLECTIONS WILL BE RESCALED ACCORDING TO 6 INDEX GROUPS

GROUP1 H=2N K=3N
GROUP2 H=2N K=3N+l
GROUP3 H=2N K=3N+2
GROUP4 H=2N+l K=3N
GROUP5 H=2N+l K-3N+l
GROUP6 H=2N+l K=3N+2

After that, Wilson statistics will be performed independently for each reflection group. This is particularly important for the automatic determination of structures having pseudo-translational symmetry, such as super-structures.

The program "PHASE" uses the RANTAN procedure [5] for phase development. In addition, it possesses a number of special features:

1. With default controlling parameters, the program will run as follows:

(1) Generate a minimum number of phase sets. This number equals 10 or the number of independent atoms, whichever is the larger.

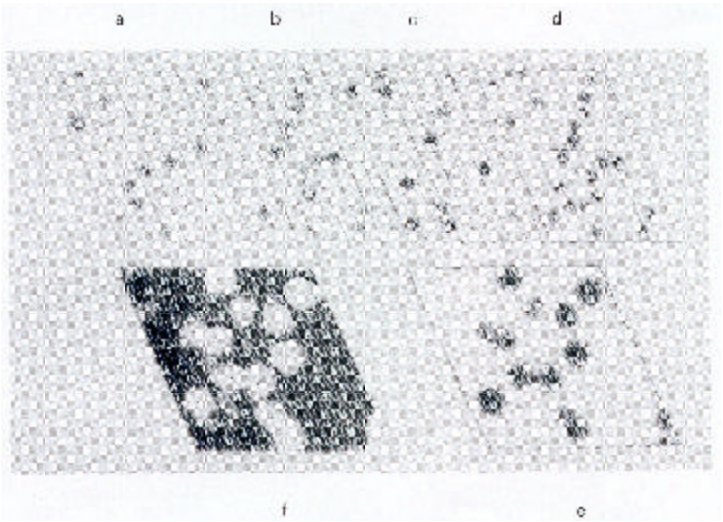
(2) After finished phase development for these sets, if none of them has a PSI (ZERO) figure of merit less than 1.6 and a RESIDUAL figure of merit smaller than 25, the program will continue to generate new phase sets up to a total number of 100 or three times the minimum number of phase sets determined according to (1), whichever is the smaller.

(3) The ordinary weighted tangent refinement will be used at first. After finished phase development for the first 10 sets, if any one of the following conditions is fulfilled, the weighting scheme will change to 'SWTR' [6] and the phase development process will be restarted.

a) The averaged absolute figure of merit greater than 1.1 and the averaged deviation among the absolute figures of merit less than 0.1;

b) The averaged absolute figure of merit greater than 1.25;

c) The averaged deviation among the absolute figures of merit less than 0.02.



a, b, and c -- sections of electron density function of ZCW;

d -- composition section consists of a, b and c;

e -- 'enlarged' map of a part from d;

f -- e with inverse contrast

Fig. 1. Typical outputs from the program "MAP".

2. "PHASE" can automatically handle a structure having pseudo-translational symmetry like this:

All triplets composed of three 'weak' reflections will be eliminated in the SIGMA2 list and the phases development will be performed in two stages. During the first stage only phases of the 'strong' reflections are developed, while in the second stage the phases of 'weak' reflections are derived by the phase relationships of the type 'weak-strong-weak'. This procedure can lead directly to a complete solution of a superstructure in favourable cases without the need of knowing the averaged (subcell-) structure.

3. In dealing with noncentrosymmetric structures "PHASE" will check each set of the final phases to see whether the averaged deviation of the three-phase invariants from 0 or π is smaller than 15 degrees. If so, the corresponding set will be recognized as a pseudo-centrosymmetric solution and warning message will be printed out.

4. If a structure model containing both enantiomorphs is input to "PREPAR", "PHASE" can break the ambiguity using the method proposed by Fan Hai-fu [4]. The result is an E-map with different peak heights for the two enantiomorphs.

Apart from E-map and Fourier-map calculations, the program "EXFFT" can calculate also Patterson maps with E-F or F^2 as coefficients. It can also perform superpositions of two Patterson maps (MPP) or superposition of an E-map and a Patterson map (MEP). MPP is particularly useful for extending a partial structure to the complete one, especially when the partial structure can not dominate the phases to give a good Fourier map. MEP can be used to eliminate the spurious peaks on an E-map making it more interpretable.

The program "MAP" prints density maps in the form of' half-tone graphs with a conventional line-printer. The program provides fully automatic control on the map size and contrast. However, user's intervention on any of the controlling parameters is possible. Fig. 1 shows some typical outputs of "MAP".