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SOFTWARE NOTICE

Adaptation to microcomputer of the Appleman-Evans program for indexing and least-squares refinement of powder-diffraction data for unit-cell dimensions

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INTRODUCTION

The computer program for refinement of X-ray powder-diffraction data of D. E. Appleman and H. T. Evans, Jr. (1973), has been used extensively by the mineralogical community since its publication. The Appleman-Evans program was designed to reduce raw powder-diffraction data, obtained from either Debye-Scherrer films or X-ray diffractometry, into a form more useful for purposes of comparison, namely lattice parameters. The program also assigns an *hkl* to each diffraction peak not indexed by the user by comparing the measured peak positions with those calculated by the program.

The Appleman-Evans program requires three essential inputs. First, the program must be given the crystal system of each sample. Second, tentative values of the lattice parameters (or parameter in the case of cubic phases) in ångström units must be entered. Last, the positions of the diffraction peaks to be used for refinement must be entered, either as 2θ angles for a specified radiation or as *d* values in ångström units.

Given these input data, the Appleman-Evans program attempts to index any peaks not pre-assigned an *hkl*. The program then proceeds to perform iterative least-squares refinements to find the lattice parameters. The program can also be used to calculate a theoretical pattern for given lattice parameters and conditions of nonextinction.

The Appleman-Evans program has been recognized as a very useful computer program for treatment of powder-diffraction data. A cursory examination of some of the most recent literature shows many examples of its application in a wide variety of mineralogical studies (Phillips and Griffen, 1986; Heubner, 1986; Černý and Chapman, 1986; Schandl et al., 1986; Payette and Martin, 1986; Moody et al., 1985).

PURPOSES OF THE REVISION

The Appleman-Evans program was designed to run on batch-processing mainframe computers. This has limited the utilization of the program inasmuch as any prospective user had to learn how to cope with mainframe operating systems. In addition, some of the geological community has little or no access to such machines. However, in recent years, less powerful but "friendlier" personal microcomputers have become commonplace. It is, therefore, opportune to adapt the Appleman-Evans program for use on such machines.

There were three somewhat conflicting objectives in the adaptation. First, it was necessary to retain as many of the computational features of the original as possible. Second, however, it was necessary to make the program as "user-friendly" as possible, i.e., a person with very limited computer expertise should be able to use the program with only minimal instruction. The last, and overriding, objective was to keep the revised program within the operational limits of the average personal microcomputer.

THE ADAPTATION

The final product consists of a package of three individual programs: BRAGG, XRAY, and XED. BRAGG prompts the user for input data and creates an input file in the proper format. XRAY is the actual Appleman-Evans program. It is important to note that no changes have been made in the computational procedures of the original program. The only differences between the microcomputer and the mainframe version of the program are file-handling procedures and changes in the output format. XED is the dedicated editor for XRAY, allowing the user to make changes in the input data file or view an output file on the screen. BRAGG and XED may be characterized as very "user-friendly" (i.e., simple to use).

USE PROCEDURES

Use of the Appleman-Evans package is straightforward. The user first runs BRAGG and inputs the raw data by following its instructions. The user then runs XRAY. The user then views the output using XED. Depending on the results, the user may then continue with another sample by running BRAGG again, or the user may revise the current data file by means of XED and then run XRAY.

SPECIFICATIONS

The revised Appleman-Evans package is designed to run on MS-DOS computers (i.e., IBM computers and the clones thereof). The computer system must have a minimum of 256K RAM memory and must have at least one floppy disk drive. An additional disk drive (floppy or hard) is highly desirable. Other peripherals, such as a dot-matrix printer, are desirable, but optional. Inasmuch as the package has been converted into executable code, no FORTRAN compiler is needed.

The entire package fits on a single 5.25-in. DS/DD floppy disk. The total size of the package is 340 000 bytes.

PERFORMANCE

The entire package has been tested extensively. The final version of the package has been tested on a variety of machines, including a Tandy 1000SX, a Zenith 158, a Zenith 241, and an IBM PC/XT. The average run time for the XRAY program, using the sample problem in the Appleman and Evans (1973) docu-

[1] Interested persons may obtain a copy of the microcomputer-based package by sending a name-brand DS/DD floppy disk (5.25 in.) to Paul Benoit or C. B. Sclar of Lehigh University. The FORTRAN source code of the entire package may be obtained by sending a second floppy disk. The package is not copyrighted and may be distributed to students or other interested persons without restriction.

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mentation, excluding the Zenith 241, is approximately 6 min. Run times range from approximately 3 to 9 min, depending on the character of the input data.

A comparison of the final lattice parameters for a sample problem from the mainframe and the microcomputer-based versions of the program is given in Table 1. The differences between the two may be attributed to the dropping of the last decimal place in some of the microcomputer calculations. Two points should be noted. First, the difference between the two sets of results is well within the standard errors. Second, the differences are well within the absolute precision limits of lattice-parameter determination by powder-diffraction methods (about 0.0001 Å) (Cullity, 1978).

TABLE 1. Comparison of program versions

	Mainframe version	Microcomputer version
a_0 (Å)	5.177 409 2 ± 0.001 427 9	5.177 419 9 ± 0.001 428 1
b_0 (Å)	8.929 532 1 ± 0.001 667 3	8.929 541 0 ± 0.001 667 5
c_0 (Å)	18.664 764 ± 0.002 730 4	18.664 770 ± 0.002 730 7
β	99°49.125′ ± 1.159′	99°49.125′ ± 1.159′

SUMMARY

The powder-diffraction-indexing and lattice-parameter-refinement program of Appleman and Evans (1973) has been adapted for use on microcomputers. The new version retains all the computational procedures of the original. As might be expected, the microcomputer version is considerably slower than the mainframe version. However, it is also much easier to use. It is hoped that this version of the program will increase the use of the refinement program and make it accessible to both professionals and students working in a variety of environments.

REFERENCES

Appleman, D.E., and Evans, H.T., Jr. (1973) Job 9214: Indexing and least-squares refinement of powder diffraction data. U.S. Geological Survey, Computer Contribution 20, U.S. National Technical Information Service, Document PB2-16188.

Černý, P., and Chapman, R. (1986) Adularia from hydrothermal vein deposits: Extremes in structural state. Canadian Mineralogist, 24, 717–728.

Cullity, B.D. (1978) Elements of X-ray diffraction (second edition). Addison-Wesley, Reading, Massachusetts.

Heubner, J.S. (1986) Nature of phases synthesized along the join $(Mg,Mn)_2Si_2O_6$. American Mineralogist, 71, 111–122.

Moody, J. B., Jenkins, J.E., and Meyer, D. (1985) An experimental investigation of the albitization of plagioclase. Canadian Mineralogist, 23, 583–596.

Payette, C., and Martin, R.F. (1986) The Harvey volcanic suite, New Brunswick. II. Postmagmatic adjustments in the mineralogy and bulk composition of a high-fluorine rhyolite. Canadian Mineralogist, 24, 571–584.

Phillips, L.V., and Griffen, D.T. (1986) Staurolite-lusakite series. I. Synthetic Fe-Co staurolites. American Mineralogist, 71, 1461–1465.

Schandl, E.S., Martin, R.F., and Stevenson, J.S. (1986) Feldspar mineralogy of the Sudbury igneous complex and the Onaping Formation, Sudbury, Ontario. Canadian Mineralogist, 24, 747–759.

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