GN m^{-2}: in very easily transformed crystals, E_{ij} may be as small as about 10 KN m^{-2}. The device described herein effectively covers the experimental range of E_{ij}.

It is a pleasure to thank R. L. Barns for discussions on constructing this device.

S. C. ABRAHAMS
J. L. BERNSTEIN

Bell Laboratories
Murray Hill
New Jersey 07974
USA

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Reference

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Meeting Report

J. Appl. Cryst. (1979). **12**, 426–427

Computer programming for protein crystallographic applications, University of California at San Diego, 28–29 November 1978

On November 28 and 29, 1978, a group of X-ray crystallographers and other interested parties gathered at the University of California at San Diego to discuss computer programming for protein crystallographic applications. This meeting was sponsored jointly by the Computer Resource for Biomolecular Research (supported by research grant RR 00757 from the National Institutes of Health) and the Department of Chemistry at UCSD. The impetus for the meeting was that several protein structure groups are currently in the process of installing DEC VAX-11/780 computers in their laboratories. This common change in computing hardware suggested to the organizers of the meeting that now would be an opportune time to establish conventions that would facilitate program and data exchange.

The participants, listed in Table 1, agreed upon a number of conventions which, since they are not restricted to VAX users alone, may be of interest to the general crystallographic community.

The topics discussed were:

(I) Magnetic tape format for interchange of data and programs in character form.

(II) Conventions for input, output, and archiving of data in character form.

(III) The structure of a binary data file (BDF) containing 'all necessary' data in program readable form.

(IV) The programming language to be used.

(V) Problems created by the lack of a standardized operating system.

(VI) The possible use of a computer network for communication and rapid exchange of programs and data.

The conventions agreed upon are:

(I) There will be two magnetic tape formats for exchanging programs and data between different installations: (1) ANSI labeled tape (ANSI, 1969) for users with compatible computers and (2) an unlabeled tape for users with dissimilar machines. These tapes may be of any track and bit density agreed upon by the corresponding parties; for the present, default shall be 800 BPI and 9 track. The following describes the unlabeled tape:

:= means 'is defined to be';
Character := USASCII/7;
Record := 80 characters;
Block := 45 records, null filled when necessary (the ASCII null character has all bits zero);
File := ⟨any number of blocks⟩ end-of-file mark;
First file := records containing the table of contents of the following files;
Tape := ⟨first file⟩ ⟨any number of files⟩ end-of-file mark.

The eighth bit of each character, the most significant bit, shall be zero. The tape is blocked with 45 records (3600 characters) in each and every block because this length is compatible with all known machine register sizes. All incomplete blocks shall be null filled in order to keep block sizes constant. The table of contents in the first file consists of the file name with no imbedded blanks, followed by a character blank and, if desired, by a descriptive comment. When all files are so described, a record of all blanks shall be present. Next may follow any number of records of descriptive text and messages. Each subsequent file, described in file 1, shall consist of filled blocks of records containing data in character form. From the definitions it is apparent that the end of tape is signaled by two sequential end-of-file marks.

(II) Because the IUCr Data Commission and various committees of the IUCr are currently seeking data formats suitable for publishing and computer archiving crystallographic data, the participants agreed that programs will have to be written to read and write data in these formats as well as in formats required by crystallographic data base systems such as the Protein Data Bank.

(III) The participants realized that adop-

Table 1. *Participants*

Richard Alden, John Cornelius, Joseph Kraut, Stephan Freer, Chris Nielson, Ng. H. Xuong, *Department of Chemistry, University of California at San Diego, La Jolla, California* 92093, *USA*.

Gerson H. Cohen, *Rm* 316, *Bldg.* 2, *National Institutes of Health*, 9000 *Wisconsin Ave., Bethesda, Maryland* 20014, *USA*.

R. E. Dickerson, T. Takano, *Division of Chemistry & Chemical Engineering, California Institute of Technology*, 1201 *E. California Blvd., Pasadena, California* 91125, *USA*.

Robert Engelmore, *Department of Computer Science, Serra House*, 26, *Stanford University, Stanford, California* 94305, *USA*.

Sydney Hall, *Crystallography Centre, University of Western Australia, Nedlands* 6009, *Australia*.

Robert Ladner, *The European Molecular Biology Laboratory*, 69 *Heidelberg, Postfach* 10.2209, *Federal Republic of Germany*.

Michael Levitt, *Salk Institute*, 10010 *N. Torrey Pines Rd., La Jolla, California* 92037, *USA*.

John McQueen, *Biochemistry Department, Wayne State University Medical School*, 540 *E. Canfield Ave., Detroit, Michigan* 48201, *USA*.

Gary Quigley, *Department of Biology* 16-743, *Massachusetts Institute of Technology*, 77 *Massachusetts Ave., Cambridge, Massachusetts* 02139, *USA*.

Michael Schmid, Lynn Ten Eyck, *Institute of Molecular Biology, University of Oregon, Eugene, Oregon* 97403, *USA*.

James Stewart, *Chemistry Department, University of Maryland, College Park, Maryland* 20742, *USA*.

Keith Watenpaugh, *Department of Biological Structure SM-20, University of Washington, Seattle, Washington* 98195, *USA*.

Alexander Wlodawer, *Reactor Radiation Division, Institute for Materials Research, National Bureau of Standards, Washington, DC* 20234, *USA*.

Richard Wrenn, *Washington University School of Medicine, Department of Biochemistry*, 660 *S. Euclid Avenue, St. Louis, Missouri* 63110, *USA*.

tion of a common method of maintaining data in an uncoded file system was essential to the 'efficient' exchange of programs. This file will be referred to as the binary data file (BDF). A detailed description of the BDF that was accepted by all participants is given by Hall & Stewart (1978). They also provide utility subroutines, written in *RATMAC* (Munn & Stewart, 1978; Kernighan & Plauger, 1976) for reading and writing the BDF. Of course, Fortran versions of these programs are available as well. The BDF is a binary blocked sequential file with self-contained blocking information. All blocks read from and written to mass storage are of equal length. The records contain two types of header information; the first is used by utility subroutines to control reading and writing the file and the second, a numeric key defined for each type of crystallographic data, serves as a table of contents to the data in the file. Several participants saw ways to expand the sequential file into scattered subfiles and recommended this as an enhancement. A complete description of the BDF is being prepared for publication by Hall & Stewart.

(IV) Although discussions on an appropriate programming language for crystallographic computing were more diffuse than those concerning data files, two points were agreed upon. First, Fortran will be the programming language because it is almost universally available, its compilers produce efficient code, and most protein crystallographers already know it. ANSI Fortran 77 conventions will be observed. Second, a structured programming language is desirable because it makes programs more readable, more transportable, easier to modify, and quicker to check out. The use of C, Pascal, Algol and other structured compliers was contemplated, but rejected. Several preprocessors which allow structured programming, but produce Fortran code for compilation, were considered and of them the consensus was that *RATFOR* and its enhancement *RATMAC,* being in the public domain, were most acceptable although their output would have to be improved somewhat to be acceptable to all present. It was suggested to Dr Stanley Hagstrom, software manager of the National Resource for Computing in Chemistry (NRCC), who was present at the meeting, that a useful project for the NRCC would be to maintain some such structured programming language.

(V) No agreement on the use of an operating system could be reached even by those with the same computer (VAX). The desirability of having a nonproprietary, standardized operating system was recognized. During discussion of this universal problem with Dr Hagstrom, the point was made that perhaps the NRCC could catalyze the production of such a general machine-independent monitor.

(VI) The possibility and usefulness of establishing a computer network for communication among crystallographic laboratories was discussed. The implications for rapid updating and the ease with which programs and data could be transfered among the groups was clearly recognized by all present; however, immediate implementation of a network was not deemed practical by a majority of the participants.

In conclusion, all participants felt that protein crystallographers would benefit, first by writing programs in a structured programming language that is converted into Fortran with a preprocessor and, second, by utilizing a common stable Binary Data File. As a result, their programs can be more widely used, have a longer lifetime, and be applicable with fewer changes to many more problems. With the advent of a new generation of computers and the development of high-level computer languages, the participants realized that now is an ideal time to standardize some aspects of protein crystallographic computing and thereby help to satisfy their collective need for reliable transportable software.

S. T. FREER

Department of Chemistry B-017
University of California
La Jolla
California 92093
USA

JAMES STEWART

Chemistry Department
University of Maryland
College Park
Maryland 20742
USA

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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).

Professor **P. P. Ewald** has been awarded the Gregori Aminoff Medal of the Royal Swedish Academy of Sciences, for his fundamental contributions to the development of the science of crystallography. This award has been established to commemorate Professor **Gregori Aminoff**, who was born in 1883 and was an accomplished artist as well as a crystallographer, having studied painting in France and Italy as a young man. Professor Aminoff was the first person to undertake X-ray crystallographic research in Sweden, in 1918. His early work included the structure determination of brucite and nickel arsenide. He was Professor of Mineralogy at the Swedish Museum of Natural History from 1923 until his death in 1947.

Dr **Isabella L. Karle**, of the Naval Research Laboratory, Washington DC, recently received an Honorary Doctor of Science Degree at Wayne State University.

Professor **Linus C. Pauling** has received the USA National Academy of Sciences Award in Chemical Sciences.

Professor **Julio Rodriguez Martinez**, Head of the Department of Geology at the Universidad Autónoma de Madrid, died suddenly in February 1979 in Santiago whilst on a visit to Chile. He did much to increase cooperation between scientists in Spain and in many countries in South America, and he was President of the Sociedad Iberoamericana de Cristalografia between 1975 and 1977. His research interests covered clay mineralogy, sediments, laminar silicates, growth of crystals and oriented crystallization. He published over 100 scientific papers and five books on crystallography. In 1973–1974 he was Honorary President of the Consejo Superior de Investigaciones Cientificas, and in 1977