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 compilers 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 transferred 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 92039
USA

JAMES STEWART
Chemistry Department
University of Maryland
College Park Maryland 20742
USA

(Received 2 February 1979; accepted 21 February 1979)

References


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, 2 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 1933 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 Autonoma 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 Cristalografía between 1975 and 1977. His research interests covered clay mineralogy, sediments, silicates, growth of crystals and oriented crystallization. He published over 100 scientific papers and live books on crystallography. In 1973–1974 he was Honorary President of the Consejo Superior de Investigaciones Científicas, and in 1977...
he became President of the Grupo Español de Cristalografía.

Professor G. A. Somorjai, of the Department of Chemistry, University of California, has been elected a member of the USA National Academy of Sciences.

Professor R. A. Young retired as Editor of the Journal of Applied Crystallography in August 1978. Professor A. Guinier has written the following appreciation of his work – Professor Young was appointed a Co-editor of the Journal of Applied Crystallography when it was created in 1968 and succeeded me as Editor at the end of 1969. He kindly invited me to continue as a Co-editor and I am happy to record what a pleasure it has been to work with him for so many years. His influence in these first years of the Journal of Applied Crystallography has been considerable and he is largely responsible for the present image of the journal: its domain is clearly distinct from that of Acta Crystallographica but its scientific standing is the same as the Union’s other publications. As a Co-editor, and still more as Editor, Professor Young has succeeded in attracting many important papers to his journal, ensuring high scientific standards with the assistance of a group of competent and devoted referees. Hence the Journal of Applied Crystallography progressively gained its now well established reputation and became, in its own specific domain, one of the main vehicles of scientific communication.

The community of crystallographers, and especially applied crystallographers, is profoundly grateful to Ray Young for his considerable and most efficient work. His departure from the editorship is regarded by everyone as a great loss, but we realise that his decision to retire was based on his generous and wise feelings for the very long-term interests of a journal to which he has become so devoted.

Book Reviews

Works intended for notice in this column should be sent directly to the Book-Review Editor (J. H. Robertson, School of Chemistry, University of Leeds, Leeds LS2 9JT, England). As far as practicable books will be reviewed in a country different from that of publication.


These two volumes of reprints of the Journal of Non-Crystalline Solids (25 and 26, 1977) contain the lectures delivered on invitation at the Xth International Congress on Glass held in Prague in July, 1977. The review articles have been written by renowned experts in the field of glass science and technology.

Volume I comprises eleven articles and is essentially concerned with glass science, i.e. the structure and properties of glasses. The first three articles describe recent theoretical and experimental studies in research on the structure of glass and its formation. The next four articles deal with various aspects of relaxation phenomena, phase separation, nucleation and crystal growth and diffusion in glasses. These papers also provide valuable information on the various applications of the results of investigations for the solution of a variety of practical problems (e.g. determination of optimum annealing schedule of glass articles, selection of optimum components for glass sealings) and for the production of new materials (e.g. vycor glass and glass ceramic materials). The mechanical and electrical properties of glasses, glass fibres as optical waveguides and physical chemistry of glass surfaces are discussed with reference to current findings in the last four articles.

Volume II includes fifteen articles. The first eleven are mainly devoted to various aspects of the technological problems of glass manufacturing processes: problems of heat transfer, design of glass melting furnaces, refractories, raw materials and batch preparation, forming machines and processes, automation and environmental pollution. One can obtain comprehensive technical information on the respective problems and related matters. In the last four articles are mentioned the diverse present and future applications of glasses – in the field of energy, in electronics, as bioactive materials, in constructional work, etc. The possibilities are numerous and exciting.

These two volumes present a good overall view of developments in research during the last decade, and will be of interest to any scientist working in these fields. Each article has also a full list of up-to-date references which will be very useful for the study of the problems in greater detail.

A. K. CHAUDHURI
Central Glass and Ceramic Research Institute
Calcutta – 700 032
India