

of the Chemical Structure Association. Assistance in preparing the syntax diagrams and checking the text has been provided by A. P. F. Cook (Orac Ltd.) and Karina Gale. Thanks are due to Dr. W. A. Warr (ICI PLC), Dr. J. D. Rayner, and Dr. M. Lord (Hull University) for helpful comments on the manuscript. Thanks are also due to the following organizations, which have provided facilities for meetings of the technical working groups: Télésystèmes Questel, Paris (June 27–29, 1988), Cambridge Crystallographic Data Center, Cambridge (July 25, 1988), Beilstein Institute, Frankfurt (November 21–24, 1988), and Molecular Design MDL AG, Basel (October 2–5, 1989). Financial support for the development of SMD Format during 1988 and 1989 has been provided by the following organizations: Bayer AG (FRG), CAOS/CAMM Center, University of Nijmegen (The Netherlands), Chemical Design Ltd. (U.K.), Chemical Abstracts Service (USA), Chemical Structure Association (U.K.), Chemodata Computer-Chemie GmbH (FRG), Ciba-Geigy AG (Switzerland), Dialog Information Services Inc. (USA), European Communities Joint Research Center (Italy), Finnigan Corporation (USA), Fisons PLC Pharmaceutical Division (U.K.), Fraser Williams (Scientific Systems) Ltd. (U.K.), Glaxo Group Research (U.K.), Hampden Data Services Ltd. (U.K.), Imperial Chemical Industries PLC (U.K.), Institute for Scientific Information (U.K.), Molecular Design MDL AG (Switzerland), Orac Ltd. (U.K.), Pfizer Central Research (U.K.), Polygen (Europe) Ltd. (France), F Hoffmann-La Roche AG (Switzerland), Sadtler Research Laboratories (USA), Sandoz AG (Switzerland), Schering AG (FRG), Smith Kline and French Research Ltd. (U.K.), Télésystèmes Questel (France).

REFERENCES AND NOTES

- (1) Bebak, H.; Buse, C.; Donner, W. T.; Hoever, P.; Jacob, H.; Klaus, H.; Pesch, J.; Römet, J.; Schilling, P.; Woost, B.; Zirz, C. The Standard Molecular Data Format (SMD Format) as an Integration Tool in Computer Chemistry. *J. Chem. Inf. Comput. Sci.* **1989**, *29*, 1–5.
- (2) Bebak, H. The SMD File Format. Version 4.3. Copies will be provided on request to Dr. W. T. Donner, Bayer AG, ZF-DID, Geb. Q18, D5090 Leverkusen 1, FRG.
- (3) Barnard, J. M. Towards a Standard Interchange Format for Chemical Structure Data. In *Proceedings of the 12th International Online Information Meeting*; Learned Information: Oxford, 1988; pp 605–609.
- (4) Barnard, J. M. Standard Representations for Chemical Information. In *Proceedings of the Montreux 1989 International Chemical Information Conference, Montreux, Switzerland, 26–28 September 1989*; Collier, H., Ed.; Springer-Verlag: Heidelberg, 1989.
- (5) Barnard, J. M.; Cook, A. P. F.; Rohde, B. Storage and Searching of Stereochemistry in Substructure Search Systems. In *Beyond the Structure Diagram* (Proceedings of a Conference held at the College of St. Hild and St. Bede, University of Durham, U.K., 17–20 July 1989); Bawden, D., Mitchell, E., Eds.; Ellis Horwood: Chichester, U.K. (in press).
- (6) Warr, W. A., Ed. *Chemical Structure Information Systems. Interfaces, Communication and Standards*; ACS Symposium Series 400; American Chemical Society: Washington, DC, 1989.
- (7) Information concerning membership of the new organization intended to oversee the development of SMD Format is available from the Administrative Secretary, Dr. Vivienne Winterman, 80 Linton Ave., Borehamwood, Hertfordshire WD6 4QY, U.K..
- (8) Brown, I. D. Standard Crystallographic File Structure. *Acta Crystallogr.* **1983**, *A39*, 216–224.
- (9) George, D. W.; Mewes, H. W.; Kihara, H. A Standardized Format for Sequence Data Exchange. *Protein Sequences Data Anal.* **1987**, *1*, 27–39.
- (10) Gund, P.; Barry, D. C.; Blaney, J. M.; Cohen, N. C. Guidelines for Publications in Molecular Modeling Related to Medicinal Chemistry. *J. Med. Chem.* **1988**, *31*, 2230–2234.
- (11) Gasteiger, J.; Hendriks, B. M. P.; Hoever, P.; Jochum, C.; Somberg, H. JCAMP-CS. A Standard Exchange Format for Chemical Structure Information in Computer Readable Form. *Appl. Spectrosc.* (in press).
- (12) International Union of Pure and Applied Chemistry, Commission on the Nomenclature of Inorganic Chemistry. *Nomenclature of Inorganic Chemistry*, 2nd ed. *Pure Appl. Chem.* **1971**, *28*, 1–110.
- (13) International Union of Pure and Applied Chemistry, Commission on the Nomenclature of Inorganic Chemistry. Recommendation for the Naming of Elements of Atomic Number Greater than 100. *Pure Appl. Chem.* **1979**, *51*, 381–384.
- (14) Mockus, J.; Stobaugh, R. E. The Chemical Abstracts Registry System. VII. Tautomerism and Alternating Bonds. *J. Chem. Inf. Comput. Sci.* **1980**, *20*, 18–22.
- (15) Cahn, R. S.; Ingold, C. K.; Prelog, V. Specification of Molecular Chirality. *Angew. Chem., Int. Ed. Engl.* **1966**, *5*, 385–415, 511.
- (16) Prelog, V.; Helmchen, G. Basic Principles of the CIP System and Proposals for a Revision. *Angew. Chem., Int. Ed. Engl.* **1982**, *21*, 567–583.
- (17) Maehr, H. A Proposed New Convention for Graphic Presentation of Molecular Geometry and Topology. *J. Chem. Educ.* **1985**, *62*, 114–120.
- (18) International Standards Organization. Data Elements and Interchange Formats—Information Interchange. Representation of Dates and Times; ISO Standard 8601, 1988.

COMPUTER SOFTWARE REVIEWS

Two FORTRAN Compilers for Microcomputers: Ryan-McFarland and Microsoft

AVI MARANI[†]

USDA, ARS, Systems Research Laboratory, BARC-West, Beltsville, Maryland 20705-2350

Received October 6, 1989

FORTRAN is one of the oldest computer languages, mainly used for mathematical and engineering applications. It is also favored by many chemists and biologists. Recently, while many scientists are using microcomputers more frequently than main-frames, FORTRAN has been replaced in many cases by other languages such as Pascal or C. There are several good

reasons, however, for using FORTRAN in microcomputers:

(1) FORTRAN has an established standard (FORTRAN 77 or ANSI X3.9-1978), so that programs written for main-frames or minicomputers can be easily transported to microcomputers and vice versa. (2) FORTRAN is the preferred language for "number-crunching" jobs, and the new 286 and 386 microprocessors (with added numerical coprocessors) can now handle this kind of job. (3) Advanced programming techniques, such as structuring, modularity, and object-oriented

[†]Permanent address: Hebrew University School of Agriculture, P.O. Box 12, Rehovoth 76100, Israel.

programming, can be used with FORTRAN 77.

The following two FORTRAN compilers for the IBM-PC and compatible machines will be reviewed: (1) RM/FORTRAN version 2.43, by Ryan-McFarland Corp.;¹ (2) Microsoft FORTRAN version 5.0, by Microsoft Corp.² These will be referred to as RMF and MF, respectively. The present version of RMF is only slightly different from the 2.40 version that was introduced in 1987. Version 5.0 of MF is new (1989) and has many enhancements to the former version 4.0. Both can be operated from two floppy diskettes, but a hard disk is preferred. RMF needs DOS 2.1 or a later version and at least 192 kB of memory. MF needs DOS 3.0 or later and at least 320 kB of memory; it can also be used from OS/2. Both compilers will run better on computers with larger memories, but they cannot use more than the 640 kB limitation of the DOS operating system.

Both compilers are compatible with the FORTRAN 77 standard, but they also have many extensions to it, such as up to 31 characters for symbolic names, INCLUDE statements, and bit processing functions. MF has all the non-standard extensions printed in blue type in the reference manual, which is very useful for writing completely portable code. MF also has compiler options to ensure compatibility with the extensions used by SAA or VAX FORTRANs. Both compilers can use the 80X87 mathematical coprocessor or an emulation library if the coprocessor is not available. They have a compiler option to produce a 80286 specific compiled program, but they cannot make full use of the 80386 chip capabilities.

RMF has a very nice programming environment called RM/FORTE, which is useful and convenient when one is working with a large programming project consisting of many files and modules. Using this environment, one can easily add or drop modules, edit program source files, compile, link, or run the program from a menu screen. I have found this environment easy to use, but the editor is not powerful enough, and I preferred to use my favorite text editor instead in many cases.

MF has introduced the "Microsoft Editor" for its new line of language compilers, and it is included in the FORTRAN

package. This is a very powerful editor, capable of block operations, macros, windows, and multiple source files, and the user can create in it new editing functions (in C or Assembly language). However, it is very difficult to learn, and a programmer who has a previously owned good text editor may not wish to invest the time and effort to learn it. The compiler can be invoked from this editor, and the error messages can be viewed, so that the code can be immediately corrected and recompiled.

Both RMF and MF have many compiler options. MF has options for handling memory models (medium, large, and huge), but the handling of these options is very complicated, and the documentation is not clear. RMF has a cross-reference option, which is very helpful for checking and analyzing a program. It is regrettable that MF does not have such a facility.

MF uses the advanced Microsoft Linker, while RMF uses PLINK86 by Phoenix Software Associates. Both linkers can link supplementary FORTRAN libraries and create overlays. Both can also interface FORTRAN and C modules, but this is quite complicated. MF has the FL facility that compiles and links in one operation.

Both compilers have a debugging option that has facilities for interrupting the program during execution and examining the value of some variables. However, programs compiled and linked with a debugging option require much larger memories, and if one tries to debug large programs (for which the debugging facility is really needed), the standard DOS memory size will be too small for this kind of operation.

The two compilers are quite fast, and they produce an efficient executable program (*.EXE) file. However, they cannot utilize the full capabilities of the 80386 processor and cannot use extended or expanded memory in DOS.

REFERENCES AND NOTES

- (1) Ryan-McFarland FORTRAN compiler is available from Ryan-McFarland Corp., Rolling Hills Estates, CA (\$595.00).
- (2) Microsoft FORTRAN compiler is available from Microsoft Corp., 10700 Northrup Way, Bellevue, WA 98004-1416 (\$450.00).