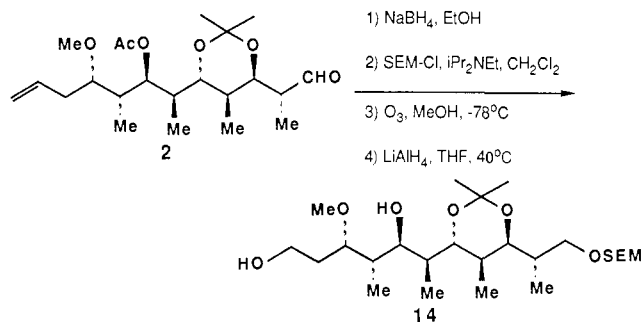


provided crude **11** that, without purification, was immediately treated with (*R,R*)-**4** under standard conditions.¹⁰ This reaction provided a 91:9 mixture of **12** and the C(27) epimer, from which **12** was isolated in 71% yield.¹² The requisite methyl ether was then prepared by treatment of a THF solution of **12** and excess CH₃I (-20 °C) with KO-*t*-Bu. Under these conditions an easily separated 8:1 mixture of **13** and the regioisomer resulting from acyl transfer prior to methylation was obtained (70% yield of **13**). Thus, protecting group chemistry was not required during the conversion of **10** to **13**. Finally, deprotection of **13** by exposure to catalytic *p*-TSA in acetone completed this 16-step synthesis of **2**.

The stereochemistry of **2** was verified by correlation with a reference sample of naturally derived **14** that was kindly provided by Professor Masamune.¹³ The two samples were indistinguishable by ¹H NMR (250 MHz), ¹³C NMR (100 MHz), IR,

(12) The combination of **11** and (*R,R*)-**4** is a matched pair. When (*S,S*)-**4** was employed, **12** and the C(27) epimer were obtained with 35:65 selectivity.

(13) Full spectroscopic data for **14** are provided in the supplementary material to ref 4f as well as in the Ph.D. Thesis of B. Imperiali (MIT, 1983).



[α]_D, and TLC analysis in three solvent systems, thereby confirming the stereostructure of **2** to be as shown.

Acknowledgment. This research was supported by grants from the National Institute of Health (GM 26782 and Training Grant CA 09112). We also thank Professor Masamune for providing a reference sample of naturally derived **14**.

Supplementary Material Available: Spectroscopic data and physical constants for all synthetic intermediates (8 pages). Ordering information is given on any current masthead page.

Computer Software Reviews *

PMR. By K. E. Gilbert and J. J. Gajewski. SERENA Software: P. O. Box 3076, Bloomington, IN 47402-3076. List price \$40.00.

PMR simulates NMR spectra for systems containing up to eight spin 1/2 nuclei. It requires an IBM PC equipped with 640K of RAM and an 8087 numeric coprocessor. Although it comes with the capability to draw crude spectrum plots on a color graphics monitor, acceptable screen plots or plots on an HP plotter required a separate program from MicroPlot, Westerville, Ohio, called PC-PLOT-III to enable a PC to emulate a Tektronix 4010 terminal. The software was also successfully tested on compatible PC's including Leading Edge Model M and Zenith Z158 running with MS-DOS 2.0 and higher. The simulation program also was run successfully on a PC-AT. The software is not copy protected and can easily be transferred to a hard disk. While no documentation is supplied, the programs are self explanatory with prompts for the necessary input. It was not difficult to use and could be used readily by anyone who has a basic knowledge of NMR spectroscopy. It is not a program to teach someone how such simulated NMR spectra are calculated. However, the source code is provided on the supplied disk. There were no problems in setting up simulation problems. Calculations for a 7-spin AA'BB'CC'X₂ system were fast. About 5 min were required both to calculate and draw the spectrum. Less complicated spectra were calculated almost instantaneously. Longer times were required for calculations of 8-spin systems. According to Serena Software, the calculations for 8-spin systems take about 30 min. Eight-spin systems were not evaluated since there is a bug in routines used for these calculations according to Serena Software. This bug has been fixed according to Serena Software, and the fix should be incorporated in current versions of this program.

Overall, this NMR spectrum simulation program is easy to use and fast. Its capabilities are greater than similar programs commonly provided with NMR spectrometers, and it is certainly adequate for the purposes for which it is intended.

David E. Bergbreiter, *Texas A&M University*

ORGANIC FONTS. By Jerry Chapman. Modern Graphics, P. O. Box 21366, Indianapolis, IN 46221-0366. List price \$79.95 (10% academic discount).

ORGANIC FONTS is a collection of three separate fonts for use with the Macintosh (512k or MacPlus) and various word processing and drawing programs. These three fonts, OrganicFont, AliphaticFont, and RingFont, are representations of many of the symbols and structural subunits that organic chemists commonly use in describing structural information. In addition, an extensive collection of Greek characters is provided in AliphaticFont. These fonts come supplied either on a 400K single-sided or 800K double-sided floppy. On the 800K version, these fonts are already incorporated within a system which can then be copied

to an applications disk. However, the size of these fonts precludes their being incorporated along with the system on the smaller capacity disk.

These fonts are accessed as any other font within a word processing or drawing application. The pulldown menu for "font" will show the addition of these three and allow their selection and use. Unfortunately, because of the rather large size of these fonts the key caps desk accessory is of limited value in viewing them, and it is most helpful to keep handy a font chart (supplied). The major use of these fonts would appear to be within word processing programs for including structural information within text lines. Although it is somewhat laborious to use these fonts in this fashion, nonetheless with experience and especially when the information is repetitive where the typist can become familiar with the key relationships, this method may save time over others that are available.

For more detailed drawing, I find the fonts quite deficient for a number of reasons. First and as pointed out by the vendor, these fonts really do not work well with the Laserwriter and although the Imagewriter does a nice job, it appears that more and more people are now availing themselves of at least access to the higher quality available from the laser printer. In addition, I find that the fonts have intrinsic difficulties with them such as their shape. For instance, the six-membered ring is not a perfect hexagon nor is the five-membered ring a pentagon. The resulting disparity in the length of the various sides of the polygons (as well as their angular relationships) led to difficulty in fusing rings together other than in the most straightforward fashion. Alternate, "perfect" pentagons and hexagons are supplied in the 18 pt size (but no 24 pt) although these print with rough appearing diagonals even on the Laserwriter with smoothing. Other structures have the same problem—that all but vertical, horizontal, and 45° lines are printed with a "stepped" appearance even with smoothing on the Laserwriter. In addition, it appears not possible to invert or rotate some of the characters without losing information, and of course, included text such as the "N" in the pyridine symbol is also rotated. Finally, the use of these fonts within framework or MacDraw (or other object-oriented drawing programs) is limited because of the inability to edit fonts within such applications. While of course various areas may be masked by, for instance, the addition of characters representing elements, the fundamental shapes cannot be varied. Thus, even if one were to use these fonts with MacDraw, one would still have to have accessible to set of rings and symbols that could be readily modified for more freehand representations in complex systems.

Overall then, I find that the fonts can be of utility within the framework of word processing applications where the time and effort required to set up a simultaneous drawing regime with switcher exceeds the value obtained from the inclusion of graphic information. Again, an experienced typist will soon learn the more common key stroke sequences necessary to include rather complex structures. On the other hand, the more complex and normal tasks of structural information are not really properly addressed by these fonts.

*Unsigned reviews are by the Computer Software Review Editor.

The manual as well as additional documentation supplied on the disk is all excellent. Tutorials for use of these fonts with MacDraw and MacPaint are supplied and should greatly facilitate learning to use these fonts.

Stereochemica. VI. Alantic Software: P.O. Box 299, Wenham, MA. List price for diskette and manual \$34.95.

Stereochemica is a disk [400K, 3.5 in.] based scrapbook of template drawing elements that are easy to combine in conjunction with MacPaint and the MacIntosh cut-and-paste (clipboard or scrapbook) routines. Written in the MacPaint format, one does not have to learn new techniques to use Stereochemica, but the accompanying manual can guide a novice MacPaint user to competent structures. The diskette illustration files are usable with the minimal MacIntosh (128K/400K internal disk drive) system and MacPaint program (ImageWriter or LaserWriter for hard copy). Additional memory, an external drive, and/or an Apple Switcher program simplify transfer of the Stereochemica-MacPaint building blocks to an opened drawing.

This enhancement of MacPaint is useful for preparing a number of simple Organic and Biochemical illustrations that are ordinarily too complex to create spontaneously in the undergraduate classroom or very

time consuming to prepare for homework or tests. Quality illustrations that supplement text book material with *another view* can easily be made on the MacIntosh system ready for conversion to a transparency, slide, or handout. The "low resolution" MacPaint illustrations prepared from the Stereochemica are not applicable to journal articles, limiting this package to undergraduate applications. It is well suited for 3-dimensional representations aiding the teaching of difficult concepts such as conformation and configuration. Critically viewing this package one must note an inherent "undergraduate" look, most noticeable in chiral formulations. Specifically, like the typical undergraduate, the Stereochemica data fail to reverse element combinations for right and left hand (bond to OH but no HO bond) representations which requires the user to create missing elements or wrongly present them in the "standard" undergraduate manner [i.e., C-HO]. Also not all of the chair and envelope forms dock without gaps. A nucleoside template is miss-drawn (both the heterocyclic and furanose systems have errors).

CONCLUSION: If one avoids computerized perpetuation of errors, applying the enhancement elements of the Stereochemica software can enrich undergraduate classroom presentations (lectures, homework, and tests).

T. A. Bryson, *University of South Carolina*

Book Reviews*

Crystal Growth. Volume 13. Edited by G. I. Givargizov. Consultants Bureau: New York, 1986. 369 pp. \$55.00. ISBN 0-306-18113-4.

"Crystal Growth" is a well-known book series that represents the English translations of the Russian book series entitled "Rost kristallov" published by Nauka Press, Moscow. As the preceding books of this series, Volume 13 is composed of a number of articles, in this case selected from presentations at the 5th USSR Conference on Crystal Growth held in September 1977 at Tbilisi. The change in editors from A. V. Shubnikov and N. N. Sheftal to G. I. Givargizov marks a redirection in the choice of articles. Judged by the exciting topics covered that for the most part are still under active study today, the new editor has been exceedingly successful with his selection although the long delay of the translation—9 years after the conference—in some cases painfully limits the impact of this book.

For example, the first article of the book, written by Boris K. Vainshtein, reviews the growth and structure determination of protein crystals and viruses. As a stimulus for enticing the traditional crystal growth community to contributing to this important field, the paper was in 1977 well ahead of developments in the western industrialized countries where professional crystal growth societies recognized the challenge only recently. Due to the substantial improvement of the speed of X-ray data manipulation by modern computers, crystal preparation has become the most time limiting step in the determination of the tertiary structure of biological macromolecules, e.g., proteins and nuclei acids. In view of the significance of structural information for progress in molecular biology and industrial developments, e.g., drug design by receptor recognition, this area of crystal growth deserves attention.

Although the presentation of Vainshtein is still of interest in this context it is somewhat outdated which holds, also, for a review of Mildvidskii and Dolginov on defect formation in III-V alloys and 3 articles by Tartachenko, Antonov, and Swek, et al., respectively, concerning meniscus controlled growth. The delay of the review by Dolginov is particularly unfortunate since his pioneering work on III-V alloys is well-known in the USA and elsewhere and stimulated in the mid-1970s the development of $Ga_xIn_{1-x}P_yAs_{1-y}/InP$ light sources and detectors for optical communications. Therefore, his paper alone, if published in time, would have assured great interest in the book by many western scientists and engineers. However, meanwhile there have been rapid advances in the understanding of III-V alloys, e.g., the recognition of critical phenomena and ordering, as well as considerable progress in processing that allows the growth of multiple quantum well heterostructures and strained layer superlattices with new effects concerning the generation and propagation of defects that are not mentioned in the review. Therefore, the paper of Mildvidskii and Dolginov is at this time totally out of touch and remains to be only of historical interest.

In spite of these short comings the book addresses many topics which have not lost in actuality. For example, a series of papers by Chernov and Ruzakin, Givargizov and Lavrentyeva et al., and Pashchenko et al.

addresses chemical vapor deposition of GaAs with emphasis on the effects of adsorption phenomena on the growth kinetics and selective epitaxy. To this are added contributions by Sokol et al., Sheftal and Klykov, Zhdanov and Medvedev, and Spitsyu, respectively, concerning the use of lattice imaging for the study of grain boundaries, graphoepitaxy of silicon, initial stages of heteroepitaxy, and crystal growth under thermodynamically metastable conditions. Also, the book contains a section entitled "New Materials' Equipment for Crystal Growth". Three articles are devoted to this topic including a review of the control of crystal growth processes by Lubl and a paper by Bagdarsarov on the use of laser heating in zone melting, pedestal pulling, and crystal growth by the Verneuil method. A particularly stimulating contribution is a paper by Rabenau on the growth of $CuTeX$ ($X = Cl, Br, I$) crystals. In the opinion of the reviewer, there is currently too little time spent with exploratory research, and including both technology related papers and fundamental research contributions is the best guaranty for creating a book that addresses contemporary problems, but retains validity over an extended period of time. G. I. Givargizov has shown considerable skill in creating such a mixture.

Klaus J. Bachmann, *North Carolina State University*

Numerical Recipes: The Art of Scientific Computing. By W. H. Press (Harvard-Smithsonian Center for Astrophysics), B. P. Flannery (EXXON Research and Engineering Company), S. A. Teukolsky (Cornell University), and W. T. Vetterling (Polaroid Corporation). Cambridge University Press: New York, Cambridge, and London. 1986. xx + 818 pp. \$39.50. ISBN 0-521-30811-9.

Numerical Recipes Example Book (FORTRAN). By W. T. Vetterling (Polaroid Corporation), S. A. Teukolsky (Cornell University), W. H. Press (Harvard-Smithsonian Center for Astrophysics), and B. P. Flannery (EXXON Research and Engineering Company). Cambridge University Press: New York, Cambridge, and London. 1986. vii + 179 pp. \$18.95. ISBN 0-521-31330-9.

Numerical Recipes is a comprehensive, practical guide to numerical analysis. It contains over 200 computer subprograms to implement the many numerical algorithms discussed in the book's 17 chapters. These computer programs are written in both FORTRAN and Pascal. Each FORTRAN subprogram is introduced by a highly informative discussion of the algorithms involved. These discussions not only present the mathematical basis for the algorithm, but the authors also incorporate the collective insight and experience of their diverse backgrounds in academia and industry.

The authors' primary theme in the book is to show "that practical methods of numerical computation can be simultaneously efficient, clever, and—important—clear". They have succeeded in their goal. For each algorithm considered, the reader is told the why's, the do's, and the don'ts. Insight and understanding not found in similar books is plentiful. The authors' discussion of random numbers is an excellent example of this. Certain innovative approaches, such as the method of simulated an-

*Unsigned book reviews are by the Book Review Editor.