

Additions and Corrections

Toward the Photostability Mechanism of Intramolecular Hydrogen Bond Systems. The Photophysics of 1'-Hydroxy-2'-acetonaphthone [*J. Am. Chem. Soc.* 1993, 115, 4321-4325].

JAVIER CATALAN* AND JUAN CARLOS DEL VALLE

Page 4321, line 6 of the abstract: The sentence should read: Despite the fact that the compound seemingly undergoes no proton phototransfer, it is more photostable than 2-(2'-hydroxy-5'-methylphenyl)benzotriazole itself ...

Computer Software Reviews

Classic Textures. Version 1.5. Blue Sky Research: 534 SW Third Avenue, Portland, Oregon 97204-9886. List price \$695.00 educational price \$495.00. Requirements: Macintosh System 6.0.4 or later; Adobe Type Manager 2.0 or later (2.0.2 for System 7); hard drive with 5 megabytes available storage; 2 megabytes RAM (4 MB recommended).

Classic Textures is a full featured implementation of Donald Knuth's T_EX typesetting program for the Apple Macintosh. It allows professional quality desktop publishing of any type of document but is particularly suited to documents making extensive use of mathematical expression. In Textures, the document editing and typesetting operations may be carried out either sequentially as with most T_EX systems or simultaneously through the use of Textures' unique "Flash Mode". This feature greatly streamlines the process of document creation and is not offered by any other implementation of T_EX of which I am aware.

A note of explanation for the uninitiated: T_EX is a software system which produces typeset documents from a plain text file with embedded typesetting commands. As such, it does not allow the free-form approach to document formatting of most modern word processors, instead granting the author the freedom to concentrate on the content of a document without expending a great deal of effort on its printed appearance. For example, the text

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\begin{displaymath}
\int_{\Omega} \{\Omega\} \{ \nabla \cdot F \} dV =
\int_{\Omega} \{\Delta \Omega\} \{ F \cdot n \} dS
\end{displaymath}
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produces

$$\int_{\Omega} (\nabla \cdot \mathbf{F}) dV = \int_{\partial\Omega} (\mathbf{F} \cdot \mathbf{n}) dS.$$

T_EX is remarkably flexible, having been used in the past for everything from Feynman diagrams to typesetting of music; it however demands a great initial investment in the learning of its syntax. Blue Sky Research thoughtfully includes copies of the L^AT_EX user's guide by Leslie Lamport and "The T_EXbook" by Donald Knuth in the Classic Textures package. Novice users may wish to supplement these with one of the many excellent tutorial books on T_EX available today.

Each document in Textures has three windows associated with it: the text window in which the source file is composed, the Typeset window in which the typeset document is displayed, and the Picture window in which pictures may be stored for insertion into the document using T_EX's \special command. When Flash mode is engaged, a small traffic light in the text window indicates the progress of typesetting. The lights are however inverted with green on top, which takes some getting used to on a monochrome monitor. In the Typeset window, the user may view the typeset document at a variety of magnifications. Holding down the mouse button in the Typeset window zooms in on a small section of the page while keeping the remainder at its current magnification. Pictures must be created by software external to Textures and pasted into a document's Picture window in order to be accessible by the document. The Picture window displays these pictures and shows their size in inches, millimeters, or picas according to the user's preference.

Installation of Classic Textures from the supplied floppy disks was straightforward, though no installer program was included with the version reviewed. According to the technical staff of Blue Sky Research, more recent versions of Textures are supplied with Apple's Installer program, which if this reviewer's experience with Installer is any indicator should make installation nearly effortless. Because Textures is supplied with 75 Computer Modern PostScript fonts, users with many existing fonts will wish to consider adding a font management utility such as Adobe Type

Reunion or Suitcase II. If no font management utility is used, fonts must be installed in the System file rather than left in their suitcases, which may present problems for applications such as word processors which build font menus. The PK font formats familiar to T_EX users on other systems must be converted in order to be used with Textures; Blue Sky Research offers free conversion utilities for this purpose. Textures is capable of typesetting with any of the Adobe PostScript fonts built into the LaserWriter Plus or II NTX printers, so the user who dislikes Computer Modern fonts has plenty of alternatives. Textures does not by default store typeset documents in the device-independent DVI format; however, it is capable of saving typeset documents separately in DVI or Adobe Illustrator format. A desk accessory is also included which produces DVI files from Textures documents for export to other systems; it can also import DVI files for viewing in Textures, although Textures, like any T_EX package, does not support direct editing of DVI files.

Using Textures is a real pleasure compared to most T_EX implementations, although a few features could be improved. The text editor is adequate; the standard Macintosh text editing operations are complemented by selectable word wrapping and indentation, but the menu and command key facilities for T_EX commands which distinguish some competing editors are conspicuous by their absence here. Another feature on my wish list is online help with T_EX and L^AT_EX commands, which would be much more expedient than the traditional approach of hunting through the manuals for each needed bit of esoterica. What Textures lacks in ease of editing is more than made up for in speed of typesetting; Blue Sky has worked hard to optimize T_EX for the Macintosh, and the results in speed are quite impressive. I tried Textures on a Mac SE/30 and found the speed to be quite reasonable albeit no match for a RISC workstation. I also tried Textures on a Mac Quadra 700 and was astonished to find that it could typeset a document almost as fast as I could type! Finally, the DVITool desk accessory does a fine job of importing and exporting DVI files; I imported a small DVI file which displayed perfectly in Textures and later exported a different DVI file created by Textures to a Sparcstation 1+, where it was converted to PostScript format and laser printed without incident. Textures itself was also observed to export DVI files flawlessly using its built in capability.

Several shareware implementations of T_EX for the Macintosh are available, of which the most widely used is OzT_EX, which can be had for a \$30.00 fee (\$150.00 for organizations). OzT_EX is much less expensive than Textures and can use standard PK and DVI files but lacks the performance and tightly integrated typesetting available in Textures.

Classic Textures is an excellent package for scientific desktop publishing on the Macintosh. Though challenging for beginners (as any T_EX implementation is), it offers sprightly typesetting performance and a tightly integrated package which the experienced user will appreciate. With a more complete text editor, this package will be just about perfect.

Epilogue: I was able to inspect a beta version of Textures version 1.6, which is in production release as this goes to press. I am pleased to report that the text editor is much improved. Word wrapping of text files can now be disabled by simply indenting a line of text with white space. This is useful for mathematics or T_EX code, which is often sensitive to line structure. In addition, the editor now supports a user-defined macros menu, which can insert often used commands in a document upon selection of the corresponding menu item. This is far more convenient than typing commands in by hand or searching through manuals to check a command's syntax. Finally, Textures now supports virtual fonts, which make it possible to create substitutions for those fonts which might be present on an output device but not on the computer. For example, if you want to send output to an APS typesetter using the Univers font but need to preview on a laser printer using Helvetica and on screen using cms10,

this facility allows you to define correspondences between these fonts. The typesetting performance of the beta version seemed as robust as the production version 1.5. These additional features are major enhancements to an already excellent package.

*Craig Blome, Department of Electrical and Computer Engineering,
The University of Texas at Austin*

SolvEq. BIOSOFT: 22 Hills Road, Cambridge, CB2 1JP, U.K.

SolvEq is a mathematics program for solving systems of equations and numerical modeling. This program requires an IBM PC/XT or AT-compatible computer with IBM PS/2, DOS 3.1 or higher and at least 512K of available memory. In order to print equations, an IBM Proprinter or compatible is required.

It would be difficult to learn how to use this program without the aid of the manual. Once a user has worked through the second chapter (about 1.5 h), the way the program functions is generally understood and the manual serves only as a reference for specifics. The format is menu driven with eight basic commands appearing on a command line at the top of the screen. An option is selected by highlighting it with the cursor and pressing **Enter**. One can leave an option by pressing **Escape**. Each option, such as **Edit**, opens as a window. In the edit window, the user can type any set of equations, usually in symbolic form, using special symbols such as integral, summation, and differential signs provided by the software. The editing process is fairly easy. When leaving the edit window the computer checks if syntax errors were made in the formulas and informs the user if he would like to change them. Upon reentering the edit window, the errors are displayed in a second window on the bottom of the screen. The equations are solved by selecting **Solve** from the command bar and the unknown values can be seen by reentering the value window. One drawback of this program is the general lack of statistics supplied. Thus it is difficult to evaluate the goodness of the fit.

The program comes with many functions built into it such as Bessel and Gamma functions, Step functions, Trigonometric functions, and Hyperbolic functions. There are also nine examples provided by the program on different problems such as a 4th order Beam equation and a parallel RLC circuit problem. These are a great help in understanding how the software requires systems of differential equations to be entered because the manual is not very clear in this area. The application has the capability of handling ordinary differential equations up to an order of ten.

The 125-page manual tries to get the user started very quickly in Chapter Two. This chapter guides the user through the basic operation of the program with simplified examples. Besides showing how the basic commands that appear on the top of the screen work, the chapter shows how to execute a parameter and an optimization study on a selected variable and how to merge different sets of equations into a unified system. This last feature allows the user to build long and complicated systems of equations in a modular fashion. This feature proved very useful in that it allowed different parts of a model to be separately debugged and analyzed. The next eight chapters each center on one of the basic commands. The final ten chapters cover specific requirements of math operations, user-defined functions, and specialties of the program.

The chapter in the manual devoted to error messages is 10 pages long and proved adequate in handling the errors that arose during the review of the software. In the section on user input errors, rather than briefly explain the error, it instead refers the reader to the chapter in the manual that concerns the error in question. It is unfortunate that the page numbers in the chapter section, instead of just the section titles, were not provided. This would have made error solving much less frustrating and time consuming on the first time through the program.

This software is a strong problem-solving tool. This quality alone is not enough incentive to distinguish a program from the many other math programs available. The ease with which this software can be learned coupled with the attractive modular design option, however, greatly increase the attractiveness of this software as an equation-solving tool for the PC.

David Coon and Andrew Bocarsly, Princeton University

FASTAT. Version 2.0. SYSTAT, Inc.: 1800 Sherman Avenue, Evanston, Illinois 60201. List Price \$495.00.

FASTAT is a sophisticated statistical package designed with the social scientist or business person in mind. It requires a Macintosh Plus or higher, running system version 6.0.2 or higher (system 7.0 compatible), and having 3.5 MB of hard drive space available and 2 MB of ram. The disks come unprotected, and one backup copy of the disk on any machine readable media is allowed.

This software accurately provides the user with various statistical analyses including Poisson and Pearson correlations, linear regression, and nonparametric statistics. In addition, there are a variety of output options, graphs, and mathematical functions available to the user. The documentation includes referenced equations and methods for the calculations performed.

For the chemist, the linear regression, ANOVA (Analysis of Variance), and the correlation functions are the most useful. Provided by the package are such useful quantities as the standard deviations of the slope, mean, and intercept. As far as the calculation of values is concerned, FASTAT does what it is purported to do.

The installation of the program is explained in documentation that resembles enclosed promotional literature; installation is not covered in the manual. Thus, most people will assume that the package follows a standard installation scheme. Indeed the installation looks fairly familiar and appears to install everything needed to run FASTAT. Unfortunately, this is not true. There are files (necessary for importing data from other applications) that must be manually placed in the System folder.

FASTAT has a poor scheme for importing data. In FASTAT there are two ways this can be done: standard copy and paste or direct importation of files. For larger files, importing the data is the best idea but the program requires a driver in the System folder. The file to be imported is merely converted into a FASTAT file, not opened, and no message tells the user that the conversion was successful. There is no dialog box that allows the user to view the text file to see how the data are delimited (tab, space, etc.). Nor is there any way to ignore a set number of lines, or to read the column titles. Unless the data are arranged perfectly, they will be converted incorrectly. The conversion is very slow, taking up to 3 min for a 3K file on a Mac IIcx running under system 7.0.

The manufacturer claims ease of use, but unless the user is an experienced statistician, much of the manual will be a learning experience. In order to use the manual, one must be familiar with the names that statisticians use for things. For example, we wanted the standard error or deviation of the slope from a linear least-squares regression. There is no listing for either of these terms in the index or table of contents. However, once we read the chapters on Linear Regression and ANOVA, we found that there was some mention of similar terms. However, comparison to the results from a program that was written specifically to calculate the standard error of the slope allowed us to resolve the terminology problem.

Regardless of the numerous output options available from the menu, the program makes little use of advanced Macintosh features. Colors are not correctly converted to gray scales when printed on a LaserWriter IIg.

Manipulating the finished graph is difficult. FASTAT treats the graph and its axes as separate items. Thus, if you click on the graph and enlarge it, the scale remains the same, and the graph is no longer correlated to the axes. In order to effect many changes in FASTAT, you are required to start your entire graph over. This is especially true for changes in the axes or the size of the graph.

The undo command is seldom available when it is needed, and there are times when you have to do something totally unrelated to undo a mistake. For example, after selecting fully factorial ANOVA, instead of Linear regression, you have to select another form of correlation to undo the ANOVA and inadvertently make the regression option available again. The undo command doesn't take the user back. Another example of starting over is that only one file at a time can be opened under FASTAT. This means that all data transfers require files to be saved and then loaded, something that renders the normal copy and paste Macintosh functions useless.

Another problem with the program is that it will simply not print anything from the view window that is larger than the page. The view window contains the output of all of the analyses. When these are printed, the far right is simply not printed. This problem is solved, if one chooses 9 point Courier for a font. A second solution might be to copy the analysis to a word processor. Unfortunately, the user is suddenly confronted by the fact that the output to the view window is all columns that have been spaced, not tabulated. Thus, the user must spend additional time sorting through the copied mess to restore the data to some readable order. The user must rearrange the data so that it can be printed.

The program has a large manual that the beginner must read in order to understand the program. This package is not one of the "install and use" variety; it requires much time to learn. It slowly performs the functions that would be useful to a chemist, and it comes with many more functions that are not useful.

*William W. West and John A. Pojman, University of
Southern Mississippi*

Axum. Version 2.0. TriMetrix: 444 NE Ravenna Blvd., Suite 210, Seattle, WA 98115. List Price \$495.00.

Axum is a technical graphics and data analysis package for MS-DOS (IBM compatible) systems. The program allows users to import data from a variety of sources, edit data, perform statistical analysis on the data, develop customized 2D, 3D contour, pie, and polar plots, and either plot the graphs on an external device or export graphs to other applications.

Requirements. The program can be installed on IBM PX, XR, ZT, PS/2, and compatible systems (Intel 80286, 386, and 486 systems). It requires DOS 3.0 or higher, 640K system memory, and 5 Mb of hard disk space. The program can be used with a wide variety of graphics cards and compatible monitors including CGA, Hercules, EGA, and VGA. The program does make use of extended and expanded memory and, in practice, more than 640K is necessary for efficient operation. A math coprocessor is recommended. While AXUM is designed to be run directly from DOS, it can be run successfully under Windows 3.0 and directly from DOS, and it can also be run successfully under Windows 3.0 and 3.1. We evaluated the program on a 80286 system without a coprocessor and a 80486 (33 MHz) with a VGA monitor. Without a coprocessor the program operates too slowly on the 286 to be of value.

Documentation. A 592 page manual is provided with the program disks. The manual is very well prepared and is well indexed. In addition, appendices are provided discussing troubleshooting, optimization, curve fitting, math functions available, slide making, and batch processing. The manual includes a tutorial on the use of the program as well as several examples of different graph types. In addition, a concise overview of all commands is given and a chapter exists discussing the Axum programming language.

Data Editor. The program makes use of stacked menus to guide the user through its various functions. A limitation is that mouse control of menu selection is not supported (Something devotees of Windows might find frustrating). The main menu directs the user to choose either their Data or Graphics editors, modify the system setup, do DOS operations, or exit the program. The data editor is very similar to that of many database programs. Data files from Lotus and dBase can be directly imported as well as ASCII and FASCII files; the routine is versatile and efficient. Data can also be generated by evaluation of a function which is typed by the user. Manipulation of blocks of data is straightforward and extremely versatile. Columns of data can be analyzed by a variety

of statistical routines including computation of a correlation matrix for a set of columns, computation of frequency distributions for a set of columns, and regression (linear, log, exponential, or polynomial) of data. The program also contains a text editor and has a programming language which can be used to operate on data, create new data, and do a variety of numeric and relational operations. The editor has functions for doing data smoothing by locally weighted regression, weighted average regression, 2D and 3D cubic spline, and Savitsky-Golay smoothing. In addition, functions exist for polynomial regression and regression of any equation that can be parametrized in a linear form. The results of statistical analyses can be displayed in columns within the database and include predicted values, residuals, etc. It should be noted that an exponential fit to 400 data points required less than a second on a 486 (33 MHz).

Graphics Editor. The graphics editor is also very versatile. To create a graph the user selects the type of plot desired from a menu and inputs columns of data to be graphed; multiple compatible plots may be placed on a single graph. Virtually every aspect of the graph sizing, labeling, ticks, colors, line widths, etc. can be specified for all the plot types supported. As stated above, a wide variety of plots can be created including bar charts, pie charts, histograms, contour and surface plots, 3D bar charts, contour plots, and many others. Once a graph is chosen and initial parameters are set, optimization of the graph may be performed using a very effective edit screen which allows complete editing and addition of titles, legends, comments, arrows, overlays, etc. Graph files can be stored in exportable formats including PIC, EPS, HPGL, GEM, TIFF, and TKF. In order to create stacked plots or arrays of plots graphs must be stored as image files (Uneditable forms); image files can be overlaid with an existing graph or a group of image files can be assembled in a specified user format. A shortcoming of the program is that it is not a Windows program so that cut and paste options are not available; the user must write a file in a format that can be read by the receiving program.

Overall, we feel Axum is a quality graphics program which is well suited for chemists wishing to produce publication quality 2D and 3D graphics. The Axum programming language makes the program useful for statistical analysis and simulation of data.

Aaron I. Baba and Russell H. Schmehl, Tulane University

Book Reviews *

Rodd's Chemistry of Carbon Compounds. Second Supplement to the Second Edition. Volume 1. Aliphatic Compounds. By M. Sainsbury (University of Bath). Elsevier: New York. 1991. xviii + 619 pp. \$85.00, \$39.95 (paperback). ISBN 0-444-88157-3.

The venerable *Rodd's Chemistry of Carbon Compounds* is at long last being updated by the issue of a second supplement. The explosive growth of organic chemistry since the first supplement in 1970 has let Rodd's recede from common use, becoming a curiosity located on the dustier of the library shelves. This second supplement is its chance to return to usefulness.

Volume 1 covers the hydrocarbons, halogen derivatives, alcohols, ethers, esters, sulfur analogs, and organometallic compounds. The nitrogen derivatives, though advertised on the cover, are postponed.

Each section covers the chemistry of that class of compounds. Occasional sections on toxicity, theoretical calculations, and physical properties come as a bonus in some sections.

Naturally, a book of this size cannot hope to be comprehensive. Whether it succeeds in its objective depends on the quality of the selection it makes and the discussion it gives. The choices made by these authors are sound. Many valuable leading references are here. In addition there are a number that will catch the eye of those who are just browsing. Discussion of the reactions are, of necessity, brief. Where the discussion is good, it is very good. A short section on the Wittig reaction is as neat an encapsulation of this process as you will find. The chapter covering aliphatic organometallics, for instance, is solid and provides a good overview of many important reactions.

Throughout the book, the references are plentiful and in the text, making them easy to locate. The index is substantial and well organized. The presentation is as good as any camera-ready format. The errors are minor and fairly few.

The second supplement will revive Rodd's. Libraries should buy it, and I think that many chemists will wish to add it to their private collections.

Roderick W. Bates, University of North Texas

Enzyme Engineering XI. Annals of the New York Academy of Sciences Volume 672. Edited by Douglas S. Clark (University of California, Berkeley) and David A. Estell (Genencor International). New York Academy of Sciences: New York. 1992. xvi + 660 pp. \$160.00. ISBN 0-89766-764-6.

This book is developed from the Eleventh International Enzyme Engineering Conference held in Keauhou-Kona, Hawaii, on September 22-27, 1991. After an introduction by the editors, there are 91 contributions organized under the following headings: Enzyme Structure and Function; Improved Biocatalysts through Genetic Engineering; Enzyme Stability and Stabilization; Novel Applications of Enzymes and Enzymelike Molecules; Enzymes under Unusual Conditions; Applications of Enzymes in Synthesis; and Innovations in Biocatalyst Preparation and Bioreactor Design. There is also a list of contributors, but no indexes.

Nuclear Magnetic Shieldings and Molecular Structure. NATO ASI Series C: Mathematical and Physical Science Volume 386. Edited by J. A. Tossell (University of Maryland). Kluwer: Boston. 1993. xvi + 584 pp. \$199.00. ISBN 0-7923-2119-7.

This book was developed from the Nato Advanced Research Workshop on the Calculation of NMR Shielding Constants and Their Use in the Determination of the Geometric and Electronic Structures of Molecules and Solids held in College Park, Maryland on July 20-24, 1992. After an introduction by the editor and a list of participants, there are 29 chapters of invited lectures and a single chapter of the abstracts of poster presentations in typescript form. There is also a short subject index.

*Unsigned book reviews are by the Book Review Editor.