Computer Software Reviews

T³—A Scientific Word Processing System. Version 2.1. T. C. I. Software Inc: 1190B Foster Road, Las Cruces, NM 88001. List Price $595 (20% Academic Discount).

For most of us word processors have changed the way we write. But as chemists the normal class of word processing programs, for all their power and versatility, fall short of meeting our needs, particularly in the areas of writing equations and chemical structures. T³ is one of a modest group of programs that have appeared in the past couple of years that attempts to meet the special needs of scientific word processing.

A reasonable wish list for such a scientific word processing program would be one which would allow the user to easily, and without too much of a learning curve, write technical reports and journal articles, prepare class handouts and transparencies, write examinations, and handle regular correspondence. A key requirement for most users would be a program that shows on the screen a very close approximation of what the final printed output will look like. That is, the scientific word processor should offer "what you see is what you get" (WYSIWYG), not just for text but for equations and chemical structures as well.

How well does T³ measure up to these ideals? The program was written by two mathematicians at New Mexico State University, Barry McKeekan and Roger Hunter, who spent a year designing the program and three more years in its development. The strong mathematical bent of the authors shows throughout T³, with its ability to handle the most complex of equations. T³ does, however, offer quite a strong set of chemical capabilities.

At the heart of the program are the alternate sets of keyboards. There are seven predefined keyboard sets supplied, which allow the generation of more than 900 characters, including mathematical and chemical symbols and italic lettering. Users can also redefine specific characters or generate whole new alternate keyboards. Two of these alternative keyboards are available at any one time (using the Alt key for selection) and others may be accessed, though in a more complicated fashion. This use of multiple keyboards provides the program with virtually unlimited character selection, but at a price. We found that remembering what each key represents was a real chore. A plastic reference chart for the main keyboard and for special command keys is provided, but other alternate keyboard selections must be printed out for reference. The program allows for the use of half-up (and down) space keys for inserting sub and superscripts, and these also work on multiple levels. Even more importantly, one can define key sequences, and it is with this feature that the program really shows its extended capabilities. For frequently used symbols, such as parentheses or brackets (which can be built up to any size and complexity), one can define special key sequences. With this special set of user defined functions one can give a sequence a special name, so that after a somewhat complex setup (that is clearly explained in the manual) one can define a letter (or word) that will write a pair of brackets of a given size, leaving one with an insert inside the brackets. All that is then needed is to fill in the appropriate fraction or formula. A set of built-up key sequences (along with the corresponding names) is available for a number of chemical and biochemical symbols. With T³ what appears on the screen is usually very close to the printed version, with the exceptions that neither character size changes nor right justification are shown on the screen. Because of its complexity, it is well that the program comes with a long and relatively thorough tutorial. The manual is adequate, but it is not outstanding. No on-screen help is available.

We found that T³ could handle almost every task of integrating equations and formulae with text that we attempted. Output on a dot-matrix printer (Epson FX-80) was satisfactory, while printing with a laser printer (Hewlett Packard LasetJet Plus) was superb (Figure 1). The one major drawback that we encountered was that the current version of T³ lacks dynamic repagination or even an on-screen line count. Automatic pagination is available at print time, but the omission of on-screen pagination makes the preparation of highly structured reports or exams a more onerous task than it should be.

For use as a normal text word processor T³ could be described as basic. It does support footnoting and multiple line headers and footlines, as well as page numbering, but it lacks a number of the capabilities of top-line business word processors, such as spelling checkers, mailmerging, outlining, multicolumn text, or multiple windows. It also does not offer the statistical features that some of the other scientific word processors in its class provide.

Dr. McKeekan reports that a revised version of T³ should be available by the end of 1986 and that this version would eliminate a number of the deficiencies of the current program. Planned changes include dynamic repagination (or at least an on-screen line indicator), a spelling checker, and mailmerging capabilities, together with a highlighting feature that will accent parts of a line.

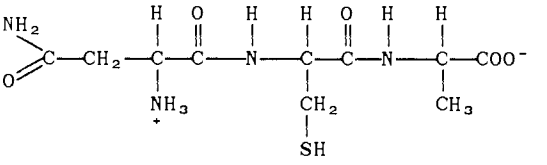

Figure 1. An example of the output of T³ on a laser printer.

T³ is operational on the IBM PC, XT, AT, and compatibles. It requires 512 K RAM, DOS 2.0 or higher, and either the Color Graphics Adaptor, the Enhanced Graphics Adaptor, or the Hercules Graphics Card. Although the program can be run with two floppy disk drives, a hard disk is strongly recommended. (The program occupies 680 K on a hard disk.) A wide variety of printers (over 40) are supported, including laser printers. One printer driver of the purchaser's choice is supplied with the program. Others are available for $60 ($90 for laser printers).

For chemists who make extensive use of equations and who are willing to take the considerable time and effort needed to become facile with this program, it is likely the program of choice amongst scientific word processors. For other chemists the choice is much more difficult. While T³ does offer a small built-in set of symbols (the amino acids, for example), most users would find it necessary to construct an extensive library of their own to make the program especially useful. It is not that T³ cannot do most of the tasks that one would like. It can. The problem is the time and effort required to make it do so. Unless there is a need for such a program on an almost daily basis then I expect that relatively few people will be willing to make these commitments. This is not a program for the casual or occasional user.

What are the alternatives? Most of the scientific word processors on the market operate in basically the same fashion as T³ and share the same set of advantages and disadvantages. A totally different approach is the use of text formatters such as PC T_EX. There are mark-up languages in which coded commands are used to control the printed output. They offer superb flexibility and control but at the expense of great complexity and a definite lack of WYSIWYG. These too are certainly not programs for the casual user. A more primitive, but effective, technique is to use a full graphics program, such as Freelance or MacDraw, to prepare structures and formulae and cut and paste these into the text.

For the time being a true WYSIWYG scientific word processor that features ease of use together with full graphics capabilities is still an unfulfilled dream. The problems of integrating keyboard use, character sets, high definition screens, and graphics capabilities, along with an ability to drive multiple printer types, remain truly daunting ones. For the moment though, despite all its difficulties of use, T³ stands at the top of the heap of scientific word processors.

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ENGINEERING TOOL KIT. By Joan Heitzeberg. Sof-Ware Tools: Boise, Idaho 83707. List Price $99.00 for MacIntosh and $59.00 for Apple II series.

Only the MacIntosh version was reviewed. Software requires Microsoft Basic Version 2.0 to be copied onto the Engineering Tool Kit prior to use. Backup copies are available at $10.00 per disk. An Imagewriter is needed for graphical output.

The ENGINEERING TOOL KIT is a collection of programs for the analysis and plotting of experimental data. In addition there are several utilities for data storage and modification, random number generation, base conversions, and a scientific calculator which appears on the screen as a hand-held calculator.

The most interesting aspect of this software is found in the data entry utility. Here one finds that two data files represent one set of x–y data, all the x values are entered in one file, and then another file is constructed for the y data. At first this seems to lend itself to a high probability that the x–y values will not be paired correctly, but this is compensated by the flexibility gained. For example, in repetitive work, the x values may be the same from experiment to experiment, thus they need be entered only once. Also, the utility allows for the manipulation of these data with a wide variety of functions. This would greatly facilitate the graphing of data for an Arrhenius, Scatchard, or Lineweaver–Burk plot where the appropriate reciprocals would be calculated rapidly by the computer.

This can be most readily done with the file structure chosen. All data may be saved on a disk and used repeatedly, or data may be entered manually for each of the following functions.

With respect to the other utilities, it is doubtful as to their usefulness. The calculator function requires too much time and effort to access as compared to using the real thing. Unless a large number of base conversions are being made, this utility will also be little used. Finally, the random number generator is not documented as to how the numbers are generated or whether or not they are truly random. The random number generator is an "open" file which the user may change to suit whatever application is desired.

Plotting of experimental data includes

Scatter Plots
Trend Plots
Histograms

In the plotting modes the program runs well although it may be considered slow by some. "Scatter plots" are defined by the author to be plots of data points with an additional regression or curve-fitting line also plotted if chosen. "Trend charts" are plots of the data with sequential points connected with a straight line with an optional linear regression line plotted if that option is chosen. Histograms or bar graphs may be generated with the addition of a normal distribution overlay if that option is selected. All plots are well designed (see below) and pleasing to the eye. Each is of a suitable size for entry into a laboratory notebook. Also, each printed plot includes a table of scaling factors, offsets, number of data points on and off scale, and regression or curve fitting data if those options are chosen.

There are some drawbacks to the plots generated. First, the graphs may be labeled and titled but subscripts and superscripts are not available and only one size plot is generated. Second, while the x axis has the label and numbering as expected, the y axis has the label on the left with the numbering on the right side. Third, data points may be represented by only squares or circles (also filled squares and circles on computers with greater than 128K of memory). Last, only 200 data points may be plotted for each graph (1000 for histograms) and only one line per graph is plotted.

Data analysis routines include

Mean and Standard Deviation
Chi-Square Test
Multiple Linear Regression
Polynomial Regression
Exponential, Logarithmic and Linear Curve Fitting
Analysis of Variation

A variety of data analysis routines are provided as listed above. Virtually no mention of the statistical methods used can be found in the manual. This is always a problem with statistics since small variations in methodology can cause considerable differences in the results. Another consideration is whether or not the routines were written to minimize rounding errors which can be significant. Linear, logarithmic, and exponential regression analysis may be plotted with the scatter plots or the results may be tabulated. A single linear regression line, least-squares line, is available with the trend plots. Multiple linear regression with up to five independent variables may be used with scatter plots, or listed as a table. Similarly a polynomial regression up to fifth order may be performed.

Completely separate from routines related to graphical plots are the Chi-square test and the analysis of variation. Chi-squared tests may be run on contingency tables from 2×2 to 4×4 in size. In the analysis of variation routine, groups of data are compared statistically to see if they are the same or not.

All of the above can be considered fairly routine programs which can be generated "in house" with a little effort. It is, however, quite convenient to have all of these in a compact, easy to run, system which can provide consistency within a given laboratory.

The 75-page instruction manual is well above par for this software. With any experience on the MacIntosh these programs are extremely simple to use. Its one drawback is that there is little reference to the calculation methods used. This package is recommended for those who would like to be able to rapidly produce graphical representations of data on a day-to-day basis. It would also be an excellent package for educational use once students have mastered the manual techniques and move on to interpretation of their data.

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Book Reviews

Enzyme-Mediated Immunoassay. Edited by T. T. Ngo and H. M. Lenhoff (University of California, Irvine). Plenum Press: New York. 1985. vii + 489 pp. $69.50. ISBN 0-306-42085-6.

During the past 15 years, there has been a proliferation of techniques for enzyme-mediated immunoassays. The literature is rich with a variety of methods for determining a variety of ligands. The review put forth by Ngo and Lenhoff offers a good overview of the theoretical aspects and basic applications of these methods. With over 560 reference citations, this book should serve as a valuable initial reference source for anyone wanting to employ the techniques or to gain general information.

In the opinion of this reviewer, the book has a few shortcomings. These are mainly in style rather than content which made it somewhat annoying, if not difficult, to read. The book is typewritten and reproduced rather than typeset. There are many grammatical and typing errors throughout the text. Some references are incorrectly cited. Several figures are not self-explanatory and require constant referral to the text by the reader for clarification. Very few graphs indicate statistical significance of data or variation in data.

The book has accomplished its intended aim—to present state-of-the-art reviews on enzyme-linked immunosorbent assays. The book would be a useful addition to an institutional library; the value of having it in one's personal library is questionable.

Richard M. Hyslop, *University of Northern Colorado, Greeley*

Biohalogenation: Principles, Basic Roles and Applications. By Saul L. Neidleman and J. Geigert (Cetus Corportion, Emeryville). John Wiley & Sons: New York. 1986. 200 pp. $49.95. ISBN 0-470-20285-8.

This book is based on the original point of view of the study of the reaction of halogenation by living organisms. It gives to the reader interesting perspectives on many different aspects of biohalogenation: the biosynthesis of halogenated antibiotics, the degradation of pesticides by microorganisms, the role of halometabolites in marine environments, the catalytic mechanism of haloperoxidases, the role of haloperoxidases in mammalian defense mechanism, and the commercial applications of haloperoxidases. Since these different fields are usually studied by specialists from separate disciplines such as microbiologists, ecologists, pharmacologists, biotechnologists, etc., this book seems to be addressed to wide audiences with the objectrive to integrate the knowledge of the various disciplines. In this perspective, it is understandable that the treatment seems somewhat superficial. I appreciated particularly how the vast catalogue of halogenated natural substances was reported and analyzed. However, I regret to find so many approximations and a lack of general perspective in the analysis of the data. For example, is it necessary to give in detail various purification protocols of haloperoxidases, without the mention of the homogeneity, the specific activities of the preparations, and the yield of the purification processes? Or is it useful to describe assays of enzymatic activity without any figures on the kinetic parameters V_M and K_M? There are weaknesses also in the part describing the defense mechanisms in man. Working hypotheses are presented like facts and minor degradative pathways are emphasized only because they pertain to halogenation. For example, the antiinflammatory drugs are presented only as potential substrates for halogenation and the degradation of the chemiotactic substances for macrophages is presented as a function of the halogenation process. In spite of all these weaknesses, I recommend this book for specialists in search of new ideas in connected fields who want a provocative perspective together with up-to-date references.

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Spectroscopy of Molecular Excitons. By V. L. Broude, E. I. Rashba, and E. F. Sheka (Academy of Sciences USSR). Springer-Verlag: Berlin. 1985. XI + 271 pp. $48.00. ISBN 0-387-12409-8.

Spectra of molecular crystals have provided significant information about both molecular and solid-state properties. This monograph describes and documents world-wide research on the latter that occurred over the last 30 years. Both experimental and theoretical results are