Computer Software Reviews

Tech*Graph*Pad. Version 2.1. Binary Engineering, Inc.: 100 Fifth Avenue, Waltham, MA 02154. List Price $275.00 and $10.00 for Demos.

Tech*Graph*Pad (TGP) is a menu driven scientific plotting and graphing program utilizing data input from Lotus 1-2-3 files, manual data input, or custom-written software (Fortran, etc.). This version is described to "run" on any IBM PC or compatible with a monochrome, CGA, or EGA monitor; 440 K of available RAM; DOS 2.0 or higher; IBM or Epson FX or LQ series printers (and compatibles); and Hewlett Packard plotters (or equivalent).

TGP was relatively easy to get running after determining that 490 K of available RAM was required rather than the stated 440 K. Consequently, the program failed to run on PC's with only 512 K available RAM since memory was also occupied by DOS leaving insufficient space for the program. Most of our evaluation was performed on an XT clone (Simplified Computer Systems, Charlotte, NC) and an IBM PS/2 Model 50, both of which had 640 K available RAM. The plotter used was an IBM 7371 2-pen unit (HP 7470A compatible). The printers were an Epson FX-86e and an Epson LQ-1000. TGP is copyrighted, but not copy protected, and therefore it is easy to place on a hard drive.

For the sake of discussion, we will compare TGP to Graph Pad (GP), a similarly priced program that we use in our laboratories and that is available from iSi Software (3501 Market St., Philadelphia, PA 19104). Both programs contain curve fitting routines and then plot the data. Both will plot on rectangular, semilog, and log–log coordinates. In addition, TGP will compute data and plot the data in polar coordinates. TGP is designed to plot multiple curves on a single set of axes, whereas GP can only plot a single curve.

TGP will perform 1st–5th order polynomial, power, and log curve fitting and cubic spline, Bazier, and Savitsky-Golay data smoothing. GP will perform most of these and many more functions unavailable with TGP. Differences were noted after performing a variety of curve-fitting and smoothing routines. TGP was much faster in determining the coefficients of equations. GP requires interaction with the user to provide approximations for curve-fitting routines (the program gives defaults) and performs from 3 to 100 iterations of these numbers to achieve the best fit for the data. In some cases, TGP visually gave totally unacceptable fits while the fits using GP appeared to be very good. Since the programs do not provide details about their curve-fitting routines, it is impossible to determine what mathematical manipulations gave rise to these observations. However, the method by which GP achieves the curves appears to be more accurate and visually the plots appear to be more appropriate.

Similar observations were found for curve-smoothing functions. Smoothing routines performed fine with both programs with the exception of the Savitsky-Golay method. In the case of data emulating a 5th order polynomial function, TGP gave totally unacceptable graphs whereas the fit produced by GP appeared to be excellent.

TGP has several modes for printing but these only work with a limited number of printers in the Epson line. One of these modes (Epson mode 3, 3″ × 3″) appears to be unusable for printing graphs. For all of the other printer options, use of Shift-Print Screen (after graphics.com is installed) gave a much more suitable graph than any of the modes in the print driver. GP can only use the Shift-Print Screen option for printing graphs since it has no print driver. However, the Shift-Print Screen Option limits resolution to that of the monitor in both cases. TGP has a Hercules mode option. However, it was not tested since our PC and PC/XT were the only computers available with the Hercules option and each had only 512K of RAM.

Graphs were also produced with a plotter. The graphs produced with both programs appeared suitable for presentations and publication, although, we would probably give a slight preference for the ones obtained with GP based on the visual layout.

In summary, TGP is a menu driven scientific graphing and plotting program. It is a very specific, self-contained package and is not readily modified for other purposes than those for which it is intended. It is fairly simple to use requiring 15–30 min to work up data and plot it. The plots are satisfactory for publication. The limitations found were related to some of the curve-fitting routines and the Savitski-Golay smoothing routine. An updated version of TGP will be released soon and it is hoped that some of these problems will be removed. The curve-fitting routines can be helpful for both academic and industrial chemists by fitting data to an equation for proper data summary and evaluation. We personally utilize programs of this type for kinetic studies and find them an invaluable tool in our research.

Randy J. Shaver and D. Paul Rillema, *The University of North Carolina at Charlotte*
Helen B. Ross, *Lithium Corporation*

GRAPH. Version 1.0. MICROMATH SCIENTIFIC SOFTWARE: 2034 East Fort Union Boulevard, Salt Lake City, Utah 84121-3144. Telephone: (801) 943-0290. List Price $79.00. Documentation plus two 5.25 in. 360K disks. Not copy protected.

GRAPH is a Turbo Pascal-3 based software program, written for the IBM, that was developed, according to the authors, to incorporate "...the most useful plotting features for scientists, while retaining a simplicity and ease of use that encourages graphical presentation of data, even in situations where it may not previously have been considered worth the effort".

Ease of use is usually inversely proportional to the range of features available, and GRAPH is no exception to the rule. However, as the developers, both of whom are chemists, point out, histograms, pie charts, and poster type graph presentation have marginal utility for the average research scientist. On the other hand, "ease of use" is exceptional with this program. GRAPH uses screen overlaid function-key menus which are, for the most part, self explanatory—a nice feature since most of us will do almost anything to avoid reading the manual.

GRAPH is basically a graphing program, but it also includes data smoothing procedures that are of considerable use. As a graphing routine, one can graph data, together with errors, entered from either the keyboard or a file, transform it in a variety of ways such as compute logs, powers, inverses, etc., and then plot the results. The graphing routine itself is quite flexible and includes the ability to add subscripts and superscripts, Greek characters, arrows, and text to the plot. The ability to "zoom" on a portion of the plot, resize, delete, and move objects at will is also a nice touch. Multiple sets of data can be displayed on the same graph for comparison purposes.

The data analysis techniques include *POLYNOMIAL REGRESSION* for inexact data and interpolation routines using *POLYNOMIALS*, *CUBIC SPLINES*, *RATIONAL FRACTIONS*, and the method of *STINEMAN*. The polynomial regression routine, run on test data by the reviewer, gave accurate results although the absence of error estimates in the expansion coefficients and the response variable is an important omission.

Once data has been entered, transformed, smoothed, etc., the results can then be transferred to either a printer or a plotter. GRAPH supports the Bausch and Lomb (Houston) DMP-029 and the HP7475 plotters and Epson, IBM ProWriter, HP LaserJet, and Toshiba 1340 printers or their emulators. The program also includes a "do it yourself" printer/plotter configuration routine. GRAPH comes configured for the Epson printer and the Bausch and Lomb plotter, but one can copy, from within DOS, other predefined drivers directly to the configuration file.

Version 1 of GRAPH supports CGA, Hercules, and the 8087 coprocessor. It is important to specify 8087 coprocessor support if desired because the 8087 version of GRAPH will run *only* on machines with this chip.

In summary, GRAPH is a relatively unsophisticated, but very useful, "friendly", and inexpensive software package that this reviewer feels is excellent value.

David W. McClure, *Portland State University*

Clue. Version 1.0. Elsevier Scientific Software: P.O. Box 330, 1000 AH Amsterdam, The Netherlands, or 52 Vanderbilt Avenue, New York, NY 10017. 1985. List price: Dfl. 975; $475.00. ISBN 0-444-42336-2.

Clue is a microcomputer program for divisive hierarchical clustering based upon the method originally developed by MacNaughton-Smith et al. Available on a single 360K diskette containing 12 files either for an IBM-PC with 128 K RAM and at least PC-DOS 2.0 or the Apple II series computers, Clue consists of three non-copy-protected BASIC programs each of which provides menu-driven option selection. Clue-A handles and edits data sets read from disk or entered from the keyboard as well as provides optional logarithmic and/or Z-transformations. The Clue user begins with Clue-A automatically, and then selects Clue-B when data are ready. Clue-B performs the cluster analysis either by objects or by variables. A dissimilarity matrix is calculated first with

either of two dissimilarity measures: Elucidian distance or correlation between data points. Alternatively a pre-calculated dissimilarity matrix can be keyed in directly or loaded from a file. The cluster analysis is performed with either screen or printer and screen display. Options exist in both programs to store new data files for each step along the way. Clue-C displays and/or prints previously stored cluster results and may be selected directly from the start-up menu.

Clue comes boxed with a vinyl, 3-hole notebook manual typical of commercial software but with oversized pages. The four-part manual includes an introduction (9 pages), user guide (79 pages), scientific background (25 pages), and program listing (39 pages). The brief introduction provides a descriptive overview and two applications. The well-written and organized user guide first describes each of the programs and menu options and then explains the simple installation procedure. Finally, operations with a tutorial data set are demonstrated, so that the user can be running Clue after only a few hours of reading. The scientific background section consists of one- or two-page explanations of each major mathematical term and procedure.

Clue can be implemented either on diskette or hard disk drive; the procedures for both are explained. A batch file (AUTOEXEC.BAT) is provided to initiate Clue-A, in which the installation program is maintained. BASICA must be available on the diskette, in the subdirectory, or through a PATH command.

The Clue programs are supplied as both BASICA interpreted (.BAS) or compiled (.EXE) files, and the start-up menu offers selection of either. As might be expected the performance of the compiled version executable file is significantly faster than the interpreted version. This becomes obvious when calculations are performed in each stage by following the displayed number of objects left to be computed. With a fast CPU (e.g., IBM PS/2 Model 80, 16 MHz), these indicators never appeared for the compiled version.

Data files are sequential with file information, including the number of objects and variables as well as missing data identifier, preceding the data. Normally, 50 objects by 50 variables can be manipulated, although changes to the source code are described to increase the number of objects (maximum recommended 65) with less variables (e.g., 25). Data entry, review, and editing are provided in Clue-A, although for large data sets, editing or configuring data files with a spreadsheet or data base management program would probably be faster and more efficient.

In no more than an afternoon a new user can be applying Clue constructively. Clue does its job well, but some additional user-oriented features would have been nice to have been included. For example, objects and variables are identified only by the order in which they appear in the data file, and the final cluster result or graphic representation (dendrogram) contains only the object numbers. If object identifiers or short labels were added to the data file and printed with the results, then the user would not have to re-identify each one during the final interpretation. Secondly, the menu selection is effective although primitive, and returning to Clue-A from Clue-B or -C requires restarting the entire program. No escape or abort is provided once some of the selections begin their operations, which makes recovering from a mistake in typing sometimes cumbersome. On the wish list of future items, it would be nice to see Clue adapted so that it could run as a command language program within a spreadhseet or data base program.

Overall, clue is a valuable and useful software package, which is easy to learn and apply. It is supported by a good user guide and reflects the long experience of the expert chemists who wrote the software.

Ramon M. Barnes, *University of Massachusetts*

*Book Reviews**

Acid–Base Chemistry. By C. W. Hand and H. L. Blewit (University of Alabama). McMillan Publishing Co.: New York. 1985. X + 273 pp. $19.35. ISBN 0-02-349910-9.

The book is not a research compendium and there are no references to the literature. It is a teaching text covering the entire range of undergraduate subject matter dealing with acid–base chemistry (some of it remotely) as taught in inorganic, analytical, and organic chemistry courses. The excellent chapters VII through IX deal in detail with the quantitative aspects of aqueous acid–base equilibria (salt hydrolysis and buffers, titrations, polyprotic and amphoteric substances). Examples of thorough solutions of numerical problems are included. Lists of problems suitable for homework or exams are given at the end of all chapters of the book.

The parts of the book dealing with what could be taught in organic chemistry contain the sort of misconceptions and pedagogically misleading aspects found in many text books—such as ground-state reasoning, careless use or misuse of the resonance concept, and failure to clearly delineate ionic compounds. The authors stretch the definition of acid–base reactions perhaps too far for useful categorization, including as examples S_N2, nucleophilic addition to C=O, and aromatic substitution. One example of a glaring error: "For diprotic strong acids [H_3O^+] is equal to twice the original molarity."

W. M. Schubert, *University of Washington*

Comprehensive Carbanion Chemistry. Part C. Ground and Excited State Reactivity. Edited by E. Buncel (Queen's University) and T. Durst (University of Ottawa). Elsevier Science Publishing Company Inc.: Amsterdam and New York. 1987. ix + 372 pp. $122.00. ISBN 0-444-42869-0.

This third volume in this series covers five diverse areas in six chapters. To my taste, the review of molecular orbital theory of carbanions by Radom and co-workers is the best, being comprehensive (at the ab initio level), insightful, and critical. The review is complete and up to date to early 1986 (392 references). Chapters 5 and 6 offer an interesting contrast in approaches to fluorinated carbanions. Koch has treated a limited number of carbanions generated by addition to alkenes and their proton transfer kinetics in alcoholic solvents. The careful analysis of isotope effects and consequent mechanistic conclusions is a model of clarity and logical thought. Chambers and Bryce have covered a wide variety of fluorocarbanions from theory through photosynthetic applications. The contributions of the DuPont group have been given scant treatment, but most references are there. Chambers makes reference to his own publications in 38 out of 128 references. The role of solvent and cation is almost ignored in this general overview. The ability of an experienced organic chemist to rationalize any trend is illustrated here.

The second chapter, by Fox, is another general treatment. It gives a broad-ranging qualitative overview of electrochemistry from the point of view of an organic chemist. The review will be of limited interest to practitioners of the art. The proof-reading of this section does not match the high standards in the rest of the volume.

Grovenstein has provided a survey and analysis of the structure of organodialkali compounds. The results of X-ray determinations and theoretical calculations are covered in detail. The importance of electrostatics and cation coordination in establishing the equilibrium structures is emphasized. Tolbert's review of the excited state chemistry of carbanions provides a sound introduction. It reveals the diversity of the area and Tolbert highlights many topics that are ripe for additional development.

This is a book for the specialist, but there are scattered nuggets here for the casual organic prospector.

John Grutzner, *Purdue University*

Vibrational Spectroscopy of Phase Transitions. By Z. Iqbal (Allied Corporation) and F. J. Owens (AMCCOM). Academic Press: Orlando, FL. 1984. x + 316 pp. $61.50. ISBN 0-12-373780-X.

This multiauthor volume reviews the application of infrared, light scattering, and neutron scattering spectroscopies to the study of phase transitions. Aside from a chapter on phase and conformational transitions in biological systems, the focus is on structural phase transitions in solids and the behavior of soft modes that couple to the relevant order parameters. There are, of course, numerous other books that cover similar material, for example, *Light Scattering Near Phase Transitions*, edited by H. Cummins and A. Levanyuk (North-Holland: Amsterdam, 1983). However, the inclusion of several, different vibrational spectroscopic techniques makes this volume rather unique, and it nicely complements the other existing reviews in this field.

The first chapter, by Z. Iqbal, reviews the basic concepts of structural phase transitions and soft modes, briefly discusses and compares the different spectroscopic techniques, and describes some selected, new developments. This chapter would be an excellent resource for researchers needing an introduction to the theory, or a succinct pointer to the primary literature. Infrared spectroscopy is discussed by J. Petzelt and V. Dvořák

*Unsigned book reviews are by the Book Review Editor.