pared by treatment of the phosphonium bromide **10**[14] with strong base, was reacted at low temperature with a solution of the dilithio dianion **13**, prepared from 2-(trimethylsilyl)ethyl acetoacetate (**12**) (Scheme II). The resulting red solution of ylide **14** was then allowed to couple with **9** to furnish (*E,Z*)-**15** as the sole diene isomer. The (*E*)-enolate of this β-keto ester was generated with high stereoselectivity by the method of Weiler[16] and was trapped with diethyl phosphorochloridate to give enol phosphate **16**. The latter underwent methylation via the magnesio cuprate[17] to produce *Z* α,β-unsaturated ester **17**. The primary silyl ether was removed from **17**, and the resulting alcohol **18** was oxidized to **19**.

Condensation of **19** with (*R*)-4-acetyl-2-oxothiazolidine (**21**) was carried out without protection of the nitrogen atom under conditions that resulted solely in crossed aldol coupling. Thus, ketone **21**, prepared directly from carboxylic acid **20**,[18] was converted to a mixed lithio cerio dianion which, upon reaction with

(13) Büchi, G.; Pawlak, M. *J. Org. Chem.* **1975**, *40*, 100.
(14) Buchta, E.; Andree, F. *Justus Liebigs Ann. Chem.* **1961**, *640*, 29.
(15) The addition of ketone enolates to **11** has previously been shown to afford ylides capable of undergoing intermolecular (Fuchs, P. L. *Tetrahedron Lett.* **1974**, 4055) and intramolecular Wittig reaction (Martin, S. F.; Desai, S. R. *J. Org. Chem.* **1978**, *43*, 4673).
(16) Alderdice, M.; Spino, C.; Weiler, L. *Tetrahedron Lett.* **1984**, *25*, 1643.
(17) Spino, C.; Weiler, L. *Tetrahedron Lett.* **1987**, *28*, 731.
(18) Maclaren, J. A. *Aust. J. Chem.* **1968**, *21*, 1891.

19, afforded an inseparable 1:1 mixture of epimeric alcohols **22** (Scheme III). Selective unmasking of the SEM ether and exposure of the resulting diol to acidic methanol gave easily separable ketals **23** and **25**. Cleavage of the ester from **23** and a Mitsunobu reaction of seco acid **24** afforded lactone **27** (mp 142–147 °C, $[\alpha]^{20}_D$ +302°), identical with the substance (mp 145–150 °C, $[\alpha]^{20}_D$ +308°) obtained by exposure of natural latrunculin A to acidic methanol. Finally, hydrolysis of **27** produced latrunculin A ($[\alpha]_D$ +143°) identical in all respects with the natural material. A parallel sequence from alcohol **25** led via seco acid **26** and lactone **28** to 15-epilatrunculin A (**29**, $[\alpha]^{20}_D$ +333°).

Supplementary Material Available: IR, ^{1}H and ^{13}C NMR, MS, $[\alpha]^{20}_D$, and analytical data for **1**, **5–9**, **12**, **15–19**, and **21–29** (6 pages). Ordering information is given on any current masthead page.

Additions and Corrections

Enzymes in Organic Synthesis: Use of Subtilisin and a Highly Stable Mutant Derived from Multiple Site-Specific Mutations [*J. Am. Chem. Soc.* **1990**, *112*, 945–953]. CHI-HUEY WONG,* S.-T. CHEN, WILLIAM J. HENNEN, JEFFREY A. BIBBS, Y.-F. WANG, JENNIFER L.-C. LIU, MICHAEL W. PANTOLIANO, MARC WHITLOW, and PHILIP N. BRYAN

Page 950: Table VI should have reaction time (min) (placed above the number 40 of entry 1), % conversion (placed above the number 49 of entry 1), and products ee (%) included.

Deoxyribose-5-phosphate Aldolase as a Synthetic Catalyst [*J. Am. Chem. Soc.* **1990**, *112*, 2013–2014]. CARLOS F. BARBAS, III, YI-FONG WANG, and CHI-HUEY WONG*

The kinetic parameters for the enzyme should be as follows: k_{cat} = 52.1 s^{-1}; K_m = 0.193 mM; and V_{max} = 55 U/mg.

Page 2014: (*S*)-1-Fluoro-3-hydroxy-4-methylhexan-2-one should read (*S*)-1-Fluoro-4-hydroxy-5-methylhexan-2-one.

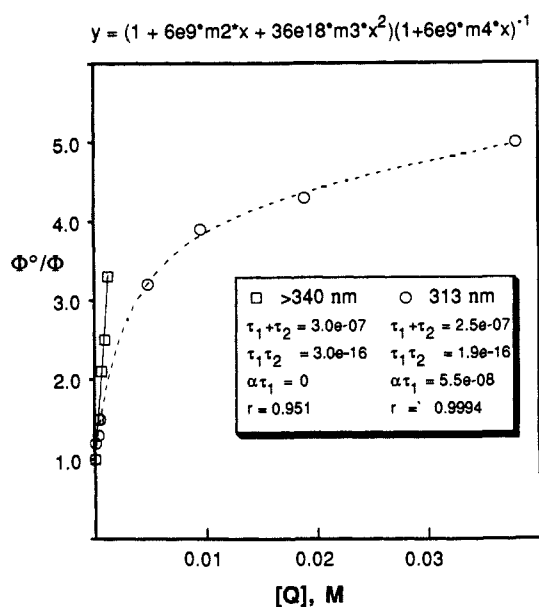# Computer Software Reviews

KaleidaGraph, Version 2.0.2. Synergy Software (PCS Inc.): 2457 Perkiomen Avenue, Reading, PA 19606. List price $249.00; educational and multicopy discounts available.

KaleidaGraph (KG) is a data analysis and graphics presentation program for the Macintosh family of computers. It requires a MacPlus or later model and System 4.1 (or later). The application itself uses 640K of memory, so 1 MB is the bare minimum RAM requirement but 2 MB seems more realistic. It claims to work with any color printer that has a Chooser print driver. For this review, it worked perfectly on an SE, a Mac II, and a Mac IIcx (all with ≥4 MB RAM); with a color monitor and a portrait monitor; and with Imagewriter II (color or black), Ima-

gewriter LQ, and Laserwriter NT printers. The program comes in two versions, for Macs with or without a floating point math coprocessor. Both versions tested ran equally well under Multifinder. The programs are not copy protected and are easily transferred to a hard disk.

KG was reviewed very favorably in the February 1990 issue of *MacUser* magazine and in the April 1990 issue of *MacWorld*. Both reviews looked at it solely as another business application, since it is loaded with facilities for making pie charts, bar graphs, and a variety of other statistical formats that rarely appear in the pages of chemical journals. I shall stress the utility of KG as a scientific application.

The program has standard, very easy to use data entry features similar

$$y = (1 + 6e9 \cdot m2 \cdot x + 36e18 \cdot m3 \cdot x^2)(1 + 6e9 \cdot m4 \cdot x)^{-1}$$

□ >340 nm	○ 313 nm
$\tau_1 + \tau_2 = 3.0e\text{-}07$	$\tau_1 + \tau_2 = 2.5e\text{-}07$
$\tau_1 \tau_2 = 3.0e\text{-}16$	$\tau_1 \tau_2 = 1.9e\text{-}16$
$\alpha \tau_1 = 0$	$\alpha \tau_1 = 5.5e\text{-}08$
$r = 0.951$	$r = 0.9994$

$\Phi°/\Phi$ (vertical axis, values 1.0, 2.0, 3.0, 4.0, 5.0)

[Q], M (horizontal axis, values 0.01, 0.02, 0.03)

Quenching of reaction from one end of a diketone

Figure 1.

to those of all good Macintosh programs. Any delimited text file can be used as input, including output from CricketGraph. (I have already changed all my data files into KG files.) Besides numerical data, which can be displayed in a variety of formats, both time and text strings can be stored in data columns. The plot menu provides a variety of choices, the most important of which are line plots and scatter plots. One can also save and later load template files that define a particular type of plot. A single plot can be created with as many as 20 dependent and 20 independent variables, with the data coming from one or more data windows. The plots can be linked to the data windows, such that any change in data is automatically reflected in the plots. Data can be masked (reversibly) so as to not be plotted. There is a Help function that succinctly outlines each menu choice, many of which have Command-key equivalents.

The program offers four important features that set it apart from its competition. First, it includes a formula function that allows users to generate data, a very useful way of comparing predicted behavior to actual data. The second outstanding feature is the ease and power of the plot formatting options. Plot dimensions are very easily altered. There is a tool box that provides standard features like erasing, pointing, arrows, and boxes, as well as a zoom window and a masking feature, both of which allow a new plot of selected data. A text tool invokes a common text editor for placing text anywhere on the plot, all of which can be printed in any font and format that the system allows. *In particular, superscripts, subscripts, and the symbol font are available.* There are many menu choices that allow fine-tuning of the plot format, including choice of symbols or error bars to represent data, precise numbering of the axes, the types of lines through the data that will be generated by curve fittings, and the color and thickness of every aspect of the plot. (I printed out a couple of plots on an ImageWriter II in which the various colors came out fine.)

It is in the curve-fitting options that the program really shines. It includes standard least-squares fits including linear, polynomial, exponential, logarithmic, power, and locally weighted, together with a cubic spline. However, the real gem is the general curve fit. Choosing this item from the menu allows you to define y as a function of x and as many as nine parameters. The program then does a non-linear least-squares fit of the data to your equation. To test this feature, I typed in an equation for a hyperbola, which I certainly have never seen in a commerical package. Figure 1 shows the results. This type of equation describes the quenching of photochemistry when excitation equilibrates between two independent chromophores. A Mac II took roughly 5 seconds to fit the data. The program operates by doing a numerical estimate of partial derivatives but allows you to be more precise by entering in the exact partial derivatives with respect to each of the variable parameters.

The non-linear least-squares fitting is done by a macrocalculator that is included as a separate feature of the program. One can call up this calculator from the menu at any time and use it exactly as an HP programmable calculator, with an eight-number stack, RPN, and a 1000-line program. KG generates the appropriate calculator program when performing any "general" curve fitting, so the user knows exactly what

mathematical algorithms are being applied. One can save these programs and alter them at will. One can also do any mathmatical manipulations required on the parameters derived from any of the curve fits.

Data and plots can be saved separately or together as one document. Macros and plot formatting styles can be saved, as can the equations used for curve fitting, together with "posted notes" for each data window, which are simply text files saying anything you want about the data. A good example would be a caption for a figure to be published, which also could be entered simply as text on the plot. Plots can be saved as PICT files, with the option to include postscript formatting information for eventual printing on laserwriters.

Printing out the plots is quite simple. One can first look at a "show page" feature which allows you to put one or more plots sized according to your specifications where you want them on a page.

All-in-all, this is an extremely powerful, relatively easy to use program for saving, analyzing, and plotting data. Each data window can hold up to 256 columns with up to 32 000 data entries in each. Up to 80 data windows and 16 plot windows can be open at any one time, given sufficient memory. The ability to define your own curve fitting and the ease of formatting plots in ways required for publication together make this a choice program. The IO interfaces conform to Macintosh standards and are therefore very straightforward to use. A 486-page manual provides a good description of all of the program's features.

Peter J. Wagner, *Michigan State University*

Un-Plot-It is a moderately priced, automated digitizing system. It runs on an IBM PC, XT, AT, and PS/2 or 100% compatible and requires the following hardware: 256K or more RAM; a Hewlett-Packard 7000 series pen plotter or 100% compatible; a monochrome or color monitor; at least one asynchronous serial communication port; and a DB25 female parallel printer port.

The Un-Plot-It package consists of a light sensor pen and box, which interfaces to a standard DB25 female printer port on the PC. The high-resolution optical pen fits directly in the pen stylus of an HP 7000 series plotter. The software included (not copy protected) is user friendly, consisting of a series of simple and logical menus which, together with the provided documentation, are very easily followed. The hardware and software installation requires only a few minutes.

Un-Plot-It digitizes in two modes: manual and automatic. The manual mode allows the user to manually move the sensor pen on the points of a graph to be digitized, after having identified the axes points: x_{min}, x_{max}, y_{min}, y_{max}, and letting the computer record their x,y coordinates. This feature can be used to identify peaks or any reference point on a graph, quickly. In the automatic mode, Un-Plot-It can digitize in either raster or line-follow modes. Raster mode can be used to digitize a scatter plot, a 3D plot, a figure, or even a photograph. In a raster scan the user defines the axes points, the upper and lower corners of the area to be rastered, and the resolution of the scan (1–10). The highest resolution possible (1) allows for a precision of 0.002 in., while the lowest resolution setting (10) uses increments of 0.018 in. The plot can be rastered at a maximum rate of 200 points/min (at 9600 baud). This transmission rate points to perhaps the only major problem of Un-Plot-It; even at the lowest resolution, raster scans of typical size figures and plots will take a considerable amount of time (hours).

Line-follow mode is used to follow a single line on a graph or plot. In this mode, the user is once again asked to identify the axes points and in addition, the thickness, endpoint, and startpoint of the line to be digitized. The same resolution scale and transmission rate mentioned above apply in this mode. Although the time required to digitize data in this mode is greatly reduced, the plot or graph must be prepared beforehand so that the line to be digitized is free of overlapping traces, grid lines, and line symbols, since any intersection between the line of interest and another line segment or a symbol will cause the sensor pen to get lost. Thus, the time gained in the digitizing process is often lost in the preparation of a graph that will be properly digitized in this line-follow mode.

In both automatic and manual modes, the digitized points are constantly echoed directly to the screen. The live, on-screen graphics is a nice feature, since it allows one to see what is being digitized. The data files can consist of up to 4096 x,y digitized data pairs and are stored in ASCII format, which allows for easy import into other applications. Un-Plot-It also has a graphing utility to plot the digitized data which includes data smoothing and a linear least-squares routine (up to a fourth-order polynomial). This graphing option is quite sophisticated and will allow the user to produce final graphs of good quality. Un-Plot-It also includes a data editor that lets the user manipulate the digitized data

in memory, and allows the addition of add new data to a digitized plot recalled from disk.

Un-Plot-It has both advantages and disadvantages. It is a fairly inexpensive package, extremely simple to set up and operate. It works reliably and accurately when the given directions are followed. However, it is considerably slow (especially in raster mode), and in the line-follow mode the graph must be "cleaned up" prior to digitization. All in all,

the best feature of Un-Plot-It is its modest price. It can be a very useful and valuable tool for those users who would like to have the capability to digitize data (i.e. spectra, chromatographs, voltammograms, stripchart, and *xy* recorder outputs) without investing a fortune on more sophisticated digitizing hardware.

G. M. Bommarito, *Cornell University*

Book Reviews *

Transport Properties of Ions in Gases. By Edward A. Mason (Brown University) and Earl W. McDaniel (Georgia Institute of Technology). John Wiley & Sons: New York and Chichester. 1988. xvi + 560 pp. $54.95. ISBN 0471-88385-9.

This is an excellent book on the kinetic theory of weakly ionized plasmas that I found to be enjoyable reading. I believe this monograph qualifies to be one of the many "classics" that should be on the shelves of most chemical physicists. I was introduced to kinetic theory in the mid-1960s, and my teacher was none other than Prof. Edward Mason. His classes were a real delight in savoring how a good scientist seeks to combine physical insight with mathematical manipulation. Mason relished emphasizing the physical aspects of kinetic theory. He loved to embellish his lectures with anecdotes from his substantial store of kinetic theory folklore. This style of teaching is one that surfaces continually even in a text as complicated as this one. I remember one beautiful example of Mason's classroom style (and by extension his writing style) where he asked us students the question which of the three laws of Newtonian physical dynamics is the law that contains the most physical content. The answer is the third law. In this case, the physical concepts of potential energy and the idea of action at a distance are invoked while the other two laws introduce definitions.

McDaniel has his own way of looking at nature that resonates readily with Mason's style. Early on, I heard a story of how McDaniel went about taking his French language exam in graduate school. Having procrastinated in preparing for the written exam, the time came when McDaniel had only a weekend to go and the whole book to study. Whereupon he purchased a bottle of French wine, a loaf of French bread, and commenced his studies in front of his fireplace. When completing the mastery of a page, he would rip it out of his book and tossed it crumpled up into the fireplace, the rationale being that this way he would be sure to learn the material. Needless to say, McDaniel went on to greater things.

It is no surprise then that the two have produced a gem of a book. The work is beautifully written and well organized. The book is a delightful mixture of penetrating discussions combining numerical and analytical mathematical techniques with relevant physical insight. Although at first glance the book may seem highly mathematically oriented, this is not really true. Quite a bit of experimental work is reviewed, and almost every page contains explicit reference to experimental result, whether as a guide in developing the theory or whether as a standard that determines how well the theoretical development might be working.

Chapters 1–4 contain the core of the experimental sections centering upon a discussion of the drift tube apparatus and the theory of analysis of the data. These introductory chapters emphasize the description of the various methods that measure ion transport kinetic parameters. The drift tube instrument, in particular, has produced important laboratory measurements of critical ion-neutral reactions that represent the core of our understanding of the interface between the weakly ionized plasma and the neutral atmosphere. Also included is a review of the laboratory techniques pertaining to the study of the afterglow which also represent an environment of weakly ionized plasma. The appendices contain a wealth of information on experimental parameters such as mobilities, transverse diffusion coefficients, transport cross sections for several model potential functions, and polarizabilities for numerous atoms and molecules. Added to this is a substantial list of data references suitable for most needs.

Then, the emphasis of the book turns to a thorough review of the theoretical developments pertaining to the calculations of the transport properties of partially ionized gases. Substantial improvements in the rigor of the kinetic theory emerged in the last 15 years, and these are all

brought together with a standard notation and the same even level of treatment throughout.

Part of the reason for this progress is that the drift tube experiment seeks to measure kinetic parameters for steady-state conditions. The thrust of the theoretical developments recognizes that for this experiment the Boltzmann equation provides too general a description. Hence, if one were willing to accept a trade of less physical information for a more precise and manageable theory, then the Boltzmann equation may be revised to get theoretical relations connecting the transport coefficients measured in the drift tube experiment with the properties of a model two-body potential. Then it becomes possible to calculate the needed parameters without having to do each and every experiment to get the necessary data.

The details of this transformation represent the heart of this book. The concept of moment equations, which represents the expansion of the Boltzmann equation with respect to the distribution function, is shown to represent a powerful method by which one can choose the level at which the physical description of the weakly ionized plasma may apply. One seeks to close the hierarchy of equations by introducing the proper basis function and truncating the series at the appropriate level. The question of the rate of convergence becomes essential to evaluating the success of the approach chosen.

Up to the middle of the 1970s, the kinetic theory of weakly ionized gases was caught up with the problems of working out these relations for nearly equilibrium situations where the distribution function is very nearly Maxwellian. This work formed the body of results that has become identified as the one temperature theory. Then a breakthrough came by reworking the theory to accept basis functions that allowed an adjustable "basis" temperature to be applied to describe separately the behavior of the ion population. This modification of the theory, designated as the two temperature theory, was greatly successful in moving the bounds of application of the theory to higher electric field strengths. Then the concept of the basis temperature was further modified and extended in a "three temperature theory" to allow for the effects of molecular anisotropy that become manifested by the behavior of these ions in the presence of an electric field.

The pathways throughout the enormous thicket of mathematical developments are well marked. Again and again, one gets the feeling of being led along these paths by an eloquent tour guide that stops at sightseeing positions along the way to point out the particular difficulties of the climb to that vantage point. Throughout, the authors take pains to bring their physical insights into play as a way of making easier the understanding of the complicated mathematical developments. In doing so, a useful tool of the narrative presentation is the embediment of dry humor that provides a nice change of pace to the flow of the narrative.

The authors are careful to point out that creativity and ingenuity are important assets in the choice of the path's continuation. Also, the authors continue to remind us that one has the computational power of the computer at one's disposal. Sometimes a sequence of complicated analytical manipulations may be necessary to reach the goal sought, but one forgets that the goal is not the elegance of the theory but to achieve a result. The authors often will point out how this goal may be achieved more readily through the computer which, for example, can be applied to provide numerical evaluations of difficult integrals easily by brute force calculations.

The book closes with a chapter on special topics relating to the applications of the several layers of the theory on gaseous transport. The ion mobility spectrometer is an instrument that uses a time-of-drift technique to separate for identification ions of different mobilities. This technique is similar to that of gas chromatography and can be quite sensitive to small traces of various species. The large ions relating to smokes and aerosols is another type of weakly ionized plasma that can

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