Additions and Corrections

Tritriptycene: A D_{3h} C_{62} Hydrocarbon with Three U-Shaped Cavities [*J. Am. Chem. Soc.* **1986**, *108*, 6675–6679]. A. BA-SHIR-HASHEMI, H. HART,* and D. L. WARD

Page 6678: Both halves of Figure 1 are identical; hence the view is not stereo. The figure shown here is correct.

We thank Dr. Silvio E. Biali (Department of Organic Chemistry, The Hebrew University, Jerusalem, Israel) for calling this error to our attention.
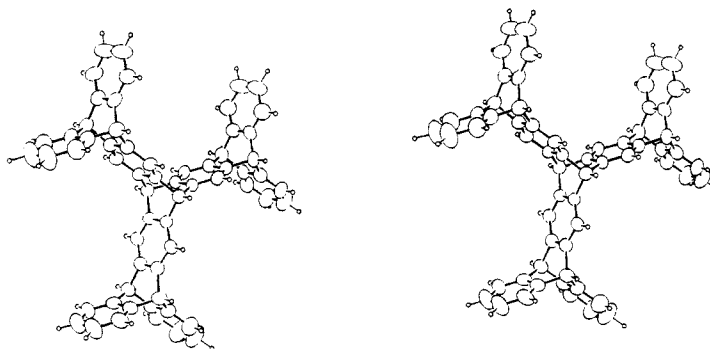

Figure 1. Stereoview of **6** (30% probability ellipsoids).

Computer Software Reviews

Temple Datatap. Graph Version 3.1 for IBM System/2, IBM-XT, AT and Compatibles. Mihalisin Associates: 600 Honey Run Rd., Ambler, PA 19002. List Price $299.00 ($199.00 academic). Comes with free technical support. Runs under Tbasic of TransEra Corp. (provided with program).

Datatap Graph is a relatively easy to use scientific graphing program which provides considerable versatility in preparing two-dimensional plots with accompanying text. It is menu-driven, which facilitates learning the package, but can be annoying when the needed functions are not in the current menu. Correctly installing and configuring the package on the computer, which requires 13 pages of the manual, is the most difficult part of using it. Subsequent loading also requires four commands, which are best incorporated into a batch file. On an IBM-AT, it required about 30 s to load and most functions were performed almost instantaneously. It can utilize the following graphics cards: IBM Color or Enhanced Color, IBM Professional, Hercules Monochrome Display, Tecmar Graphics Master, AT&T or Olivetti M24, HP-45981, HP-45983, and Artist 1, 1+ and 2. Screen color with the IBM-CGA reverts to black and white below the first menu level. Plotter drivers include the following CalComp, Houston Instr. DMPL, Hewlet Packard HPGL (and plotters such as the Sweet-P 600, which use HPGL), Tektronix 4662 and 4663. According to the manufacturer, the HP Laserjet runs very slowly with this package, but will function adequately with additional software available from Insight Development Corp., Miraga, CA. A number of GPIB controllers are also supported. Graphs can also be printed on an IBM Graphics Printer or any 24 pin printer with an Epson LQ emulation.

Once installed, much of the package can be learned without referring to the manual. In fact, the manual is fairly cursory and difficult to use, since it does not reference page numbers, but rather function keys in a hierarchical command tree structure, some of which are referenced to manual pages. Useful on-line prompts are provided and often one must use a combination of these, the table of contents, the index, and one's own intuition to solve a particular problem. When all else fails, the telephone support from the manufacturer is very helpful in clarifying particular points.

The package is a useful adjunct to laboratory data acquisition and analysis programs, such as ASYST, which are limited in their graphic capabilities. Data are easily imported directly from Lotus or Symphony files, Ascii files, or simply keyed in. Data can also be stored as Ascii files. Previously stored graphs or data files are readily accessible, even in other directories or disk drives. HPGL files can be stored as such, plotted outside of Datatap, and sent through electronic mail networks. Greek characters, an array of mathematical and graphics symbols, subscripts, and superscripts are all available in a range of sizes. Scaling can be automatic or specified. Automatic conversion to log or exponential scaling is provided. Tic marks and numbering on axes, line types, pen color, and frame size are all variable. Axes can be moved to any number on the axes. Default axes labels can be specified by the user or custom labels added for each graph. Up to 15 titles and labels can be placed anywhere on the graph and rotated to any angle.

In the present version, sorting of the data can only be accomplished in an ascending fashion, and this only by going to the plot/alter menu, plotting the data as a bar graph, returning to the previous menu, and refreshing the graph. Error bars are adjustable for any data point and may be presented symmetrically or asymmetrically, with or without the cross line, or only in one direction. Data may be fitted as a straight line or as up to a sixth order polynomial and the values of any individual point calculated. An applications note indicates that other functions are available by using one of several "alter variable" commands; however, the available functions for fitting are still limited. Since it is not the purpose of the package to provide a general nonlinear regression facility with error analysis, this will most often by done by a separate data analysis package and the results plotted with Datatap Graph. A programmable area of code is available for transforming the data in TBasic. Data smoothing of the Y-variable is available as a weighted three point moving average; however, this may cause the axes to be repositioned. Either linear or cubic spline fits are available to fit single-functioned data; however, subsets of the data cannot be spline fit independently.

A multiframe facility is available so that up to 9 graphs can be accessed, and plotted as insets or in arrays. Temporary "metagraphs" can

bc stored on disk and are deleted on leaving the program. Any portion of the graphs may be plotted or printed independently.

In general, this is a fairly powerful plotting package, which researchers will find useful in presenting two-dimensional data. Desired features, such as sort functions and an improved manual, should be added in future versions and the relatively few bugs eliminated.

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Data Desk (Professional Version). Odesta Corporation: 4084 Commercial Avenue, Northrbook, IL 60062. List price $175.00 with 220-page manual.

The Data Desk is a useful statistical data analysis and data display software package for Apple Macintosh personal computers (with at least 512K memory and 800K disk storage). Several statistical analysis packages for Macintosh systems have appeared; the Data Desk is an easy-to-use and learn, and user-friendly, system that appears to be similar to the StatWorks package reviewed previously (*J. Am. Chem. Soc.* **1988**, *110*, 16552). The diskette provided is not copy-protected, so that back-up copies can be made and the system can be transferred to, and run from, a hard disk.

Data Desk operates via the familiar Macintosh desktop with pulldown menus and icons. The user can perform data analysis without having to learn a new computer language or sets of commands. An inexperienced user, who is familiar with the Macintosh, can learn the basic features and use the program in an hour or two. Variables (containing the data in the form of numbers or text) are represented as icons whose contents can be displayed, plotted, or moved to other Macintosh applications via the Paste command and the Clipboard. Data are easily entered and edited in a word processor-like style and can be imported from other applications, such as spread sheet programs. The variables can be grouped into bundles, which facilitates the manipulation of large data sets.

Data Desk contains the usual range of statistical tools and procedures. The mean, median, midrange, beweight, standard deviation, interquartile range, variance, maximum, minimum, and other statistics can be computed. It can perform simple inference tests, e.g., t-test and z-test for individual means, two-sample t, chi-square test, F-test, etc. Almost any type of statistical analysis that would be of interest to a chemist (and many others which probably would be of less use) are included. The package provides for simple and multiple linear linear regression analysis, but not for direct nonlinear (polynomial) regression (e.g., by spline techniques). This is probably one of the greatest weaknesses of the program for use by chemists in analyzing data. The system does provide for easy transformation of data, however, and this may allow some results

to be cast in a form that can be analyzed via linear least-squares procedures. Data transformation is carried out by defining a new variable in terms of other variables via an algebraic formula, and allows the usual arithmetic, trigometric, log, exp, and round-off functions, and a number of statistical (collapsing) ones. Data can also be sorted and ranked and random numbers can be generated from uniform, normal, Bernoulli, Binomial, and Poisson distributions.

We were particularly impressed with the speed and plotting abilities of Data Desk. Data can be displayed graphically as histograms, x–y (scatter) and x–y–z (rotating 3-D) plots, and box plots. This can be printed on an imagewriter or laser printer from within the Data Desk, or exported as MacPaint files that can be altered, edited, and printed via that application. The current version of Data Desk allows only a single point size and shape in the plots. An updated version is promised which allows for other point symbols as well as overlay of the plots (which is not possible with the current version). The scatter and 3-D plots could be readily manipulated via the mouse-driven controls. The zoom-in and zoom-out features and the speedy rotation of the 3-D plots were especially helpful. We also found that the Data Desk was useful for generating sets of data and plotting various functions. A set of numbers over an arbitrary range with any spacing can be generated with the "generate patterned data" command and then transformed algebraically and plotted in only a few minutes.

The Data Desk Handbook is very clear and easy to read. It not only describes how to use the program, but also provides tutorials on the meaning of the various statistical functions and when they can be used. Numerous exercises are included to allow the interested reader to learn more about statistics and the capabilities of the package. A number of practice data sets (e.g., Michelson's measurements of the velocity of light in air and the fat content of eggs) are provided for use in these exercises and to practice on the various features of the program. A user can learn a lot about statistics, relatively painlessly, simply by going through the handbook and playing with the program. A less-expensive, smaller, student version of the program is also available.

Overall, the Data Desk provides a user-friendly environment for the management, analysis, and display of data via a program that is easy-to-learn and use. A number of statistical analysis and plotting programs are now available for microcomputers. The best course of action in selecting one would probably be to try several out and select one at a level and with the features appropriate for the type of data usually handled. The Data Desk is certainly one of the packages that should be considered.

Note: Version 2 is now available from the vendor at a cost of $495.00 (academic discount available) with 600-page documentation. The vendor has indicated that this version has substantial enhancements for graphics, statistics, and data management.

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Book Reviews

Infrared Spectroscopy: Analytical Chemistry by Open Learning. By W. O. George and P. S. McIntyre (Polytechnic of Wales, Pontypridd). John Wiley and Sons: Chichester and New York. 1987. xx + 537 pp. $36.95. ISBN 0-471-91383-9.

The text of this book is divided into two major sections. The first is a discussion of infrared instrumentation and the theory of the interaction of infrared radiation with matter. This section also includes a part on sample preparation and handling. The second part of the text deals with the interpretation of infrared spectra. Spectral interpretation starts with simple systems and develops into the interpretations of complex spectra. The text is essentially a workbook. Explanations of principles are provided to the reader, and then a few exercises are given on each section. The answers to the exercises are provided in the text immediately after the questions are posed. The exercises are often followed by Self-Assessment Questions (SAQ). In the SAQs, these questions are generally more detailed than the short exercises, and the answers are provided in a separate section at the end of the text. The overall organization of the book is very good. The electromagnetic spectrum is introduced first, followed by classical and quantum theory of vibrational and rotational spectroscopy. The introduction is completed with a discussion of the distribution of lifetimes of energy states and vibrations of polyatomic molecules. The second chapter of the book explains instrumentation for infrared spectroscopy. This is followed by sample handling which ends the first half of the text. The second half, as stated above, deals with

spectral interpretation. A general guide to infrared spectra and spectral regions is provided. The next topic is hydrogen bonding and how it affects infrared spectra. A chapter is then introduced on quantitative analysis. Perhaps this chapter is a little out of sequence. The last chapter, and the largest, deals with spectral interpretation. According to the preface of this book, it was written for students who do not necessarily have a formal university training. This appears to be equivalent to a technical degree in the United States (the first two years of college or university). Although the intent of the book is for self study, it would probably be very valuable as a supplemental text at the undergraduate level. This book provides an excellent source for many practical problems in interpretive infrared spectroscopy and provides a very good workbook format for students to learn basic skills. It is undoubtedly very valuable for anyone who wishes to acquire basic skills in infrared interpretation. The authors point out that much of the first part of the book, specifically that part referring to instrumentation, is highly subjective. As a reviewer I must agree. I found that some of the instrumentation arguments were slightly out of date, and the emphasis is not what I would choose were I to write a similar text. Nonetheless, I found the interpretive part without flaw. For that reason I would strongly recommend that instructors of infrared interpretive spectroscopy seriously consider this book as a supplemental text.

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