

be 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, Northbrook, 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 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, trigonometric, 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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