Additions and Corrections

Theory of Vibrational Circular Dichroism: trans-2,3-Dideuteriooxirane [J. Am. Chem. Soc. 1988, 110, 2012-2013]. K. J. JALKANEN, P. J. STEPHENS,* R. D. AMOS, and N. C. HANDY Page 2013: Reference 11 should read as follows—Freedman, T. B.; Paterlini, M. G.; Lee, N.; Nafie, L. A.; Schwab, J. M.; Ray, T. J. Am. Chem. Soc. 1987, 109, 4727.

Computer Software Reviews

Picture Perfect. Version 4.0. Computer Support Corporation: 15926 Midway Road, Dallas, Texas 75244. List Price \$295.00.

A majority of us work with graphical information every day. We use it to visualize research data, determine kinetic parameters, prepare presentation material for meetings, classes, and reports and provide figures for publication. In all these areas, microcomputer programs can greatly facilitate the preparation of graphs. Recently there has been a flood of graphics programs for IBM and compatible microcomputers coming to the market. Most of these are aimed at the business world. As chemists, our needs generally differ substantially from that audience. We have little use for organizational charts, Gantt and Pert plots, or high/low and three-dimensional exploded pie charts, which are common features of most business graphics programs. By contrast, we typically employ a range of curve and scatter plots. Desirable features would include the ability to both use and import large data sets, automatic scaling, multiple X and Y axes, the ability to use both semilog and log plots, several types of statistical analysis, and curve fitting procedures and output options that allow quick rough figures on dot-matrix printers, as well as publication quality graphs on plotters and laser printers.

PicturePerfect is a middle-of-the-road business graphics program. It offers bar, line, combined bar/line, and pie charts. Multiple charts per page are available and both log/log and semilog plots are supported, as are two independent Y axes. The program operates on IBM PC/XT/AT and a variety of compatible computers equipped with 512K of RAM memory and a graphics card (including VGA). An extensive listing of printers (dot-matrix, inkjet, and laser), plotters, and film devices is supported, but no provision is provided for the use of a mouse or for print queing of graphs.

PicturePerfect works under a DOS-shell system called C-SAM that provides a common access point for the Computer-Support Corporation's family of programs (see the accompanying review for Diagraph). The PicturePerfect program is supplied on 9 diskettes (including C-SAM) and is something of a memory hog. It occupies approximately 2 megabytes on a hard-disk, not including the C-SAM module. While the program can be run with floppy-disks only, this requires a lot of disk shuffling. Alternatively, the program runs with C-SAM as a key-diskette in a floppy drive and other files on a hard disk. The program allows installation and operation on a hard disk, without using a key diskette, but only a single installation is available from the master disk. A back-up diskette is available free upon registration of the program. The program can be uninstalled to the master disk to provide a means to reinstall the program on another computer. This copy protection scheme certainly serves to foil multiple, illegal installations of the program, but is unnerving if one has experienced the tribulations of hard disk failures. In today's world of copy protection free programs, PicturePerfect is an anachronism. Installation on a hard disk is relatively straightforward, but does involve the removal of any terminate and stay resident (TSR) programs, such as Sidekick, before installation

All the major operations of the program are accessed through the function keys, using a nested series of commands. The general system is quite easy to master, but it is far from intuitive and involves quite a lot of maneuvering through the submenus. A context-specific on-screen help system is available at any time and is very useful in learning the program. The manual consists mainly of an extended tutorial, which in itself is quite good, but it is frustrating to use as a general manual and

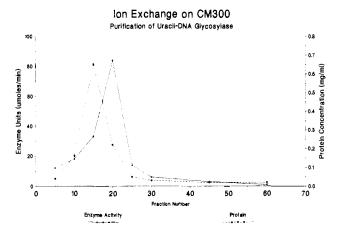


Figure 1.

more detailed technical information would be of great assistance. Without a math co-processor, screen redraws seemed interminable, even though the program was tested on a 12 megahertz AT class machine. There is no charge for technical support, although the call is not toll-free.

In the line-graph mode, PicturePerfect can handle 8 lines of 200 data points each and 9 types of line patterns are available. Any of the keyboard characters or 7 types of bullets can be used as data points. No sizing of these data point characters is allowed and this results in obscuring of the points if larger line widths are employed. The graphs can be just lines or include data points and labeling of data values. Only point-to-point lines are available and no provision is made for any curve smoothing techniques or data analysis. One deficiency was that the position of X and Y axis labels could not be readily adjusted. The program is able to import data files in ASCII or DIF format. Thirteen different typefaces are provided with the program and others are available as options. These typefaces can be shared with Diagraph. The quality of output on a dot-matrix printer is quite satisfactory for nonpublication uses (see Figure 1), although printouts of even quite simple graphs can take 10 min or more. With a plotter, first-rate graphs were obtained.

The current version of PicturePerfect has a considerably improved front end menu system compared with previous releases and the program now provides for exchange of data and other chart information between different types of graphs. One still has to go through the tedium of exiting the current application and reloading a chart file if one wants to swap between, say, a bar graph and a pie chart. No chartbook is offered and there is no slideshow option. This latter omission is sorely missed, since it is very helpful in putting together oral presentations. Surprisingly, there is no means of integrating graphic images from the companion program Diagraph to dress up PicturePerfect charts. Computer Support Corporation also offers PicturePerfect and its companion program Diagraph in Windows versions. This has the great advantage of allowing the swapping and integration of graphical and pictorial information between programs.