

## Additions and Corrections

**Theory of Vibrational Circular Dichroism: *trans*-2,3-Di-deuteriooxirane** [*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 queuing 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

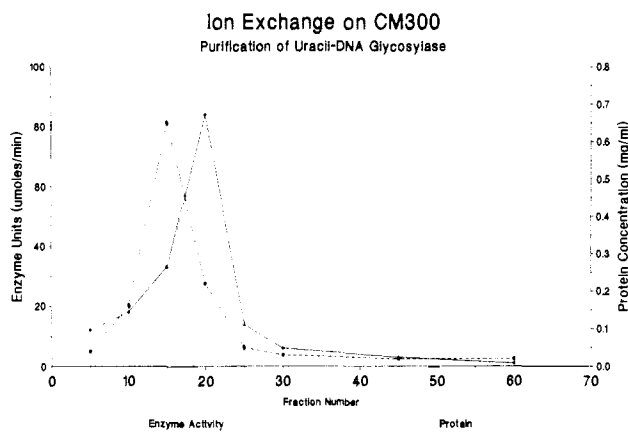


Figure 1.

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 non-publication 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.

In summary PicturePerfect can be rated as an adequate though not outstanding business graphics program. It lacks a number of the features and flexibility of some of the top end competition, like Harvard Graphics. For scientific graphing it comes up short in several areas, most notably in the lack of ability to do any curve smoothing in line graphs or to perform even the simplest statistical analysis of data.

G. Barrie Kitto, *The University of Texas at Austin*

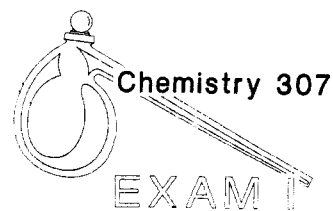


Figure 1.

**Diagraph. Version 4.0.** Computer Support Corporation: 15926 Midway Road, Dallas, Texas 75224. List Price \$395.00.

At heart, Diagraph is a very large clip-art library, with the ability to size images, stretch and rotate them, and fill them with a variety of shading patterns. These images can then be combined with other images from the library and with text. As with any such library, the utility of the program depends upon the number of images available and their suitability for the task at hand.

The program comes with a library of more than 2000 well-drawn images and symbols, and more than 3000 others, including maps, are available in optional library packages at prices ranging from \$59.00 to \$129.00. Thirteen type faces are provided and twice that number are available as options at a cost of \$25.00 each. The symbols range from a vast array of graphic aids such as arrows (more than 250 different kinds), banners, boxes, and word balloons to signs and icons such as road signs and transportation symbols as well as pictorial representations including trees, buildings, clouds, and perspective composition aids. The program is designed to run on IBM PC/XT/AT and compatible systems. It operates most conveniently on a hard disk and a math coprocessor enhances the speed of the program considerably.

Diagraph operates under a common shell-management system with PicturePerfect and suffers from the same antiquated copy protection system. The program comes on 9 diskettes and occupies about 2 megabytes of space on a hard disk. Like PicturePerfect, the menus and submenus as well as most editing functions are accessed through the function keys. Sizing and other manipulations of images would be greatly enhanced if mouse support was provided. Any text included in an overall chart has to be attached to a image or icon and this occasionally causes problems, since when an image is deleted from a chart any associated text is also eliminated.

Diagraph supports an exceptionally wide range of printers, plotters,

and film recorders. Output on dot-matrix or laser printers is more than adequate, but multicolor printing with a plotter or conversion to high resolution slides really shows the capabilities of the program to its best advantage. Diagraph is an object-oriented program, rather than a raster-based paint program. This has a multitude of advantages for precision work. File sizes are small and high resolution is maintained over a very wide range of image size and when objects are rotated and/or sized in a nonproportional manner. Moreover, the resolution of the final image is independent of screen resolution and is limited only by the hardcopy output device. Image editing is also greatly simplified compared to raster-based programs. Unfortunately, cutting and pasting of images into other programs, such as PicturePerfect, is not available—except in the Windows version of Diagraph.

Using Diagraph, it is a snap to create report covers and announcements since the images and text can readily be scaled from  $1/8$  in. to several feet. The author has found the program very useful for generating posters, exam covers and transparencies for use in class (see Figure 1).

The Achilles' heel of Diagraph is that it does not offer users any abilities to create images from scratch. While the library has a very large range of images, one is often left frustrated by an inability to find exactly what one needs. One can modify the library images and text faces in size and shape almost endlessly, but this is not the same as having free-form capabilities. Custom made libraries and logos are offered as a service by Computer Support Corporation, but for most users the cost and time delay would be prohibitive. If the program offered the drawing capabilities of packages such as Lotus' Freelance Plus or Micrografx Designer, the combination with a large symbol and icon library would be a winner. Illustration of chemical structures in any desired size range is just one of the examples that comes to mind.

In short, Diagraph offers an exceptionally large graphics library, but it is emasculated to a considerable degree by the lack of drawing facilities.

G. Barrie Kitto, *The University of Texas at Austin*

## Book Reviews

**Color Chemistry: Syntheses, Properties, and Applications of Organic Dyes and Pigments.** By Heinrich Zollinger (Swiss Federal Institute of Technology). VCH Publishers: New York. vii + 367 pp. \$110.00. ISBN 0-89573-421-4.

This is a timely, incisive, and user-friendly book on preparation and uses, both conventional and modern, of organic dyestuffs. It is expressly intended for organic chemists who may view color chemistry as a closed topic, color chemists who may not be aware of new trends and new technological uses of dyes, and physical chemists confused by the vastness of the field. The reviewer falls in the third class, and found himself with six pages of closed-spaced notes on topics and references for immediate examination upon completing the review process.

The first ten chapters deal with the major classes of dyes, their synthesis by ecologically favorable methods, and the modern view of their unique features. Two central chapters on dyes and pigments (microcrystalline materials) describe dyeing, dye aggregation, and the physical states of pigments from the view of modern physical chemistry. Three chapters focus on the dynamic behavior of dyes and, implicitly, on the transition to active dyes which DO something in high technology. These active aspects include photosensitized reactions, photochromism, harvesting of solar energy by dye systems, dye lasers, and modern image-forming systems. The book closes with a chapter on biomedical staining and a short chapter on ecological topics. The user-friendly quality of this book is enhanced by its compactness and disciplined quality. It is in no way a historical or classical view of the dyestuff industry, and the 21 pages of references focus on key review articles and on intellectual transition papers of whatever age. All the right review references are

there!

This book is, of course, a labor of love for the author. Inevitably one of the high points is the chapter on azo dyes, coming as it does from his own continuing research interest. One can regret the compact format, which prevented all but a brief account of the author's own work on the use of zinc-complexed azo dyes as long wavelength sensitizers for ZnO electrophotographic materials and seems to have prohibited any discussion of the use of nigrosines and other ionic dyes as charge-control agents in electrophotographic toners. Also missing is an account of use of dyes in photodynamic therapy, in which some diseased or malignant tissue is selectively stained with a sensitizing dye to facilitate laser removal of the material. Comments have been made on the very low efficiency of solar photogalvanic systems and on the low efficiency (to date) of the two-dye water-electrolyzing systems such as Ru(bpy)<sub>3</sub> and dimethylviologen. An omission especially significant to this reviewer is the topic of solid state solar photovoltaic cells employing organic dyes as the active components. Major projects on organic photovoltaics have been conducted in at least three major industrial laboratories, and efficiencies have been obtained which mark the best of the organic photovoltaics as potential competitors to amorphous silicon (Loutfy, Morel, Chamberlain, Tang). From the standpoint of a very conservative dyestuffs industry, the missing ingredient for the 21st century is a large volume, high technology application of photoactive dyes of this sort.

Among many candid and incisive comments is a remark about vat dyes: "It seems that this area of research for textile applications is saturated." In context this remark is to be contrasted with an earlier discussion of new and ecologically acceptable syntheses for azo dyes, work