

Additions and Corrections

Multiphoton Infrared Photoinduced Ion-Molecule Reactions in the Gas Phase [*J. Am. Chem. Soc.* 1993, 115, 737-742]. YONGQING HUANG AND BEN S. FREISER*

Pages 739 and 740: In the printing process, the two figures shown over figure captions 2 and 3 were reversed.

Computer Software Reviews

Origin 2.0. Scientific Graphics and Data Analysis in Windows. MicroCal Software Inc.: 22 Industrial Drive East, Northampton, MA 01060. US price \$495.00 (academic users \$400.00; student \$199.00). Software author: Dr. C. P. Yang.

This program was tested with Windows 3.1 and two IBM clones, both 80386 machines running at 33 MHz and having 80387 numerical coprocessors. One had a VGA monitor and the other a non-interlaced 1024×768 monitor with a Compaq advanced graphics board (now perhaps rather antiquated). Either computer is a suitable machine for adequate use of Origin and I believe Origin would work reasonably well with slower machines but I did not see the need nor have the time to test this aspect. Origin 2.24, the actual version tested, seems designed for Windows 3.1 (which most users probably have by now) although Microcal is willing to ship a Windows 3.0 help file if required.

Origin is in many ways a superb program and seems to possess practically everything one could possibly wish to use for scientific graphics of numerical data. Output on an HP Laserjet III with and without a Postscript cartridge and also on a 24 pin dot matrix printer was more than adequate. In some ways however, there are more features than I feel I could ever use including a very versatile script programming language called "LabTalk". I would like to find the time to use the script but, so far, the built-in features have sufficed. Perhaps, like some well-known word processing programs, the student edition, a more limited version, might be easier to use. I certainly found it necessary to go through the very complete tutorial to obtain an understanding of the program and I am sure that I have learned to use other programs more rapidly.

The program is basically a worksheet with associated layers of graphical windows and has many impressive and useful features: high performance mathematics, very versatile curve-fitting, controls on all aspects of printing (e.g. thickness of lines, colors, fonts etc.), enlargement of one part of a graph, and superposition of graphs in adjustable-sized windows. I was impressed by the provision of a screen reader to read the cursor position, the ease of switching between different data worksheets, and the availability of templates. A template can also be made from any graph that a user has drawn. It is not specifically mentioned but incorporation of textual material from any Windows word processor is relatively easy using the clipboard.

The features which seem to make Origin stand out over previous programs are numerous. The ability to mix sizes, colors, and styles in captions is impressive although the manual did not explain font shifts and the information had to be obtained from MicroCal's technical assistance (actually my phone call was returned the next day by the program's principal author Dr. C. P. Yang). Scale control in graphs is very flexible and includes ready introduction of axes breaks. The worksheet and the graph are linked dynamically, and the mathematical functions available are quite complex as are curve-fitting functions (extending to multiple Gaussians of considerable utility for chromatograms). Plotting and printing are relatively easy; one can operate on a limited number of data e.g. applying a mathematical function to a subset of rows in the worksheet. Manipulation and editing of graphs is remarkably easy with the provided tool palette especially shifting and sizing legends.

The program, in the nature of things, is not perfect and there are aspects which one would like to see improved. The column captions are sometimes slightly overlapped by other details on the monitor, "UNDO" is not available as often as one would like in editing, some textual materials declared as the same style and font do not have the same size on the monitor, when a column is added the worksheet window does not expand automatically and has to be pulled open in the usual Windows fashion, the "magnification tool" is difficult to use, and reversion to a previous screen is tricky. In editing graphs it is sometimes difficult to get the cursor in position to "click" on a line. There are one or two spelling errors on the screen notably "drivation" during fitting. One useful improvement would be a consistent place for the OK button in dialog boxes. I seemed

to spend a considerable amount of time trying to find buttons and, in fact, finding items in the many very crowded dialog boxes was very slow although I suppose one would learn as one used the program. However, programmers should always remember that even programs such as Origin are used intermittently as adjuncts to research and a readily remembered user interface is a great advantage.

In summary, I consider this elaborate program to be the best available Windows Scientific Analysis program and would recommend it to any scientist despite its rather formidable price. I do not suppose that specialized programs of this type will ever achieve the sales of word processing programs, and thus the cost may be justifiable. It probably should be stated that the views expressed are my own and do not commit NIH in any way.

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DISKEEPER/Plus, Version 6.0. Executive Software: 701 North Brand Blvd., 6th Floor, Glendale, CA 91203-1242. 1992. List price \$320.00-13200.00.

DISKEEPER/Plus is a customized on-line disk defragmenter which runs under the VAX/VMS operating system. It converts fragmented files to contiguous ones and also consolidates free disk space. The defragmenter package includes the application on a MT, 8 mm, RX50, or customer supplied TK50 and documentation which describes the installation and operation of the defragmenter. The minimum hardware needed to support DISKEEPER/Plus is any DEC supported VAX/VMS system with VMS Version 5.0-5.5. Installation of the software requires 5000 blocks on the system disk, and 2000 blocks are needed on the disk where the product files will reside. Additionally, DISKEEPER/Plus uses 600-800 blocks of physical memory; however, 1000-1200 blocks may be required for badly fragmented disks.

The defragmenter offers a wide array of operational features. These features allow each defragmentation job to be customized to the users exact specifications. The user has the option to create jobs from either a command line interface or a menu system. The menu commands can be stored in macros for fast recreation of defragmentation job specifications. DISKEEPER/Plus also has default setups that take the guesswork out of customizing by simplifying the selection of the numerous qualifier options. The simplicity of DISKEEPER/Plus allows the user to have a "set it and forget it" approach to disk defragmentation. After the initial creation of the job specifications, disk defragmentation will run on that specific schedule indefinitely without further maintenance. Once a job is set up, defragmentation of disk space will not interfere with users accessing files on the same disk and will also automatically determine the optimum run frequency to prevent disks from becoming fragmented again.

DISKEEPER/Plus has many fail-safe features that are designed to protect the data files during the defragmentation process. One of the ways the defragmenter ensures this is by using only a single I/O instruction that replaces the original file pointers with the new defragmented file pointer. This guarantees that the entire defragmented file is intact. Another feature of this utility is the files are directly copied from the original to the new location without intermediate copies. DISKEEPER/Plus also uses the VMS read-check and write-check capability on every I/O to ensure data integrity.

DISKEEPER/Plus is an efficient disk defragmenter that virtually eliminates the need to backup and restore data. The cost of the defragmenter package varies with each system configuration and is partially justified by the improved performance of the system. DISKEEPER/Plus is a very useful VAX/VMS system tool and should be considered by the appropriate scientific community.

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