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Additions and Corrections

Electron Transfer vs Polar Mechanisms. Transition-State Structures and Properties for Reactions of a Cation Radical and a Nucleophile [*J. Am. Chem. Soc.* **1991**, *113*, 9890]. JEOUNG KI CHO and SASON SHAIK*

The $\Delta S^{\ddagger}$ value for the ET process in Table I should be −28.7 eu. The relevant discussion in the text was based upon this value and therefore there are no changes in the conclusions of the paper.

Does the Mechanism of Symmetric Methyl Transfer to Water from Water Differ from That for Transfer to Water from Other Leaving Groups? [*J. Am. Chem. Soc.* **1989**, *111*, 792]. JOSEPH L. KURZ* and MICHAEL W. DANIELS

Recent measurements show that the values reported in this communication for the isotope effect and rate constants are not correct. We (H. S. Yathirajan and Joseph L. Kurz) plan to submit an article providing details after we have completed our investigation of these rates and isotope effects.

Computer Software Reviews

PEAKFIT. Version 3.01. Jandel Scientific: 2591 Kerner Blvd., San Rafael, CA 94901. List price $595.00.

The proliferation of and utility of varied forms of spectroscopy coupled with the now general availability of desktop computers makes sophisticated data analysis a real part of many projects. In many cases, deconvolution of overlapping signals through the use of nonlinear equations and curve fitting is an application of computers which potentially provides useful qualitative and quantitative information. Peakfit by Jandel Scientific is an IBM PC-based software program designed as an aid to researchers with an interest in using nonlinear equations and curve-fitting procedures in data analysis.

Peakfit constructs and evaluates components of a peak outside the boundaries of the instrumental resolution. For example, we used the review copy to resolve overlapping peaks from NMR spectra, IR spectra, and XPS (X-ray photoelectron) spectra. The main requirement is simply that the spectral data be available in a digital format, most commonly in an ASCII format for importation into the program. The program features rapid, high quality, nonlinear curve fit procedures. The program offers an excellent graphical/numerical review for a critical evaluation of the fit. A variety of different curve-fit procedures are available either as standard analytic functions or as user modified functions.

Peakfit is written for IBM compatible computers. The program is operated in a windows-like environment using pull-down menus with either a mouse or keyboard commands. It is compatible with windows but does not run as a windows application. A hard disk is required and the program uses about 1.9 Mb of hard disk. The program supports VGA, EGA, MCGA, Hercules (Monochrome), ATT, IBM 8514, or IBM PC-3270 graphics. A math-coprocessor is highly recommended. Without a coprocessor, the program is too slow to be useful. We tested the program on various brands of 80286, 80386, and 80486 computers and experienced no major compatibility problems. This program runs as a DOS application under Windows.

Using the program revolves around four steps. First, the X–Y data table is either entered or imported from another source. This is followed by the users choice of functions in such a way that the sum of the functions approximates the data. The program then performs an iterative curve fit to obtain the best fit. The user then evaluates the fit graphically and numerically. Finally the output is sent to a printer or as a file according to the users choice.

Data input/output is versatile. Besides ASCII import, you can automatically read in files from several sorts of spreadsheets. Manual data entry is also possible. Calculation options include a variety of arithmetic functions which can be used to modify these values in a manner like that used with common spreadsheets. Portions of the data can be selected and ignored to facilitate analysis. Data imported as an ASCII file can include a maximum of 32 000 points with 5 MB of Virtual Memory (can be any combination of expended, extended, RAM, or hard disk memory). With 640K of RAM and 256K of Virtual Memory (can be simply hard disk space), a maximum of 3000 points can be included in the data set.

The next step is to approximate the data to a function. Several application families such as spectroscopic, chemical-pharmacological, waveform, and statistical applications ease the selection of the proper function. Multiple functions can be used to fit a given set of data points. A known parameter can be fixed during the process of curve fitting. User-defined functions further broaden the utility of the standard built-in functions and provide for added flexibility. Choice of a particular function is followed by curve fitting. Curve fitting occurs with a visual update after each iteration as the program searches for a best fit. Curve fitting can be aborted if desired to change one or more parameters. At the users discretion, the visual updates can be suppressed to speed up the calculations though speed was not a problem on the machines we used.

The curve fitting is followed by a graphical review displaying the original data, the constituent functions, and the sum curve. A graphical display of the residuals gives a better idea about the closeness of the fit. Apart from the graphical review, a numerical review enables one to analyze the fit for each individual point. In cases of unsatisfactory fit, alternative functions can be chosen to improve the fit or parameters can be adjusted and curve fitting used again.

The curve-fitted data can be printed to most dot-matrix printers, HP LaserJet printers, HPGL plotters, etc. The fitted data can be exported to other programs such as Lotus-123 and SigmaPlot 4.0 or exported to HPGL or metafile format. Postscript output is also possible.

A manual is provided which is comprehensive and takes the user through a total tour of all the functions and capacities of this powerful software. A chemist with some computer experience should be able to sit at the keyboard with the manual and would feel at home with the software in a few hours. The powerful program stimulates further research and challenges the user to import more complicated problems to