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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

be solved by the program. Jandel provides an 800 number for technical support as well as a number for a BBS.

The program presents to the user a set of functions that would normally be foreign to most chemists and which could be intimidating to people with an ordinary mathematical background. However, since the program emphasizes the use of these functions as tools in a graphical environment, this potential problem is largely if not totally minimized. Peakfit appears to be a very powerful program with genuine utility for data analysis. Anyone who needs to use curve-fitting procedures would find the program very useful. We know of no other comparable program that offers such sophisticated data analyses with such a simple, straightforward interface.

David E. Bergbreiter and Balasubramanian Srinivas, *Texas A&M University*

NanoVision. Version 1.0. ACS Software: American Chemical Society, 1155 16th Street, NW, Washington, DC 20036. List price $295.00. ACS member price $245.00; educational price $265.00.

NanoVision is a fully-integrated molecular graphics program designed for Apple Macintosh computers. The software can import chemical structures stored in a binary file format as well as a variety of common text file formats including Brookhaven Protein Data Bank, Cartesian, Chem3D Cartesian, Alchemy II, CONCORD, and Moldat files. Once entered, these structures can be viewed in a variety of styles including wireframe, ball and stick, and space filling. NanoVision is very user friendly and allows complete control of molecule orientation, atom and bond color, bond thickness, shading, and van der Waals sphere diameter. The software also allows the user to easily create stunning animations utilizing its capability to record structures one frame at a time to disk and then play them back rapidly.

The program will run on any Apple Macintosh computer with 1 MB RAM and System 6.0 or later system software. (For this review, NanoVision was evaluated extensively on a Macintosh PowerBook 170 with 4 MB RAM running System 7.0 operating software as well as on a Macintosh IIx to evaluate the color and animation capabilities.) A hard disk, math coprocessor, and 2 MB RAM are recommended. NanoVision comes with a 84-page user manual and technical support is provided through the ACS Software Technical Support Desk. NanoVision can manipulate structures of up to 32000 atoms and has a variety of features that allows one to work with these large structures easily, including a grouping feature, a clipping feature, and a mixed-style presentation feature. The grouping feature allows the user to "define" a group of individual atoms or groups of atoms within complex structures for quick and easy manipulations. This part of the software is particularly user friendly, allowing one to personalize the group selection as well as the use of the protein structure information contained in the Brookhaven Protein Data Bank files as predefined groups. The clipping feature allows one to temporarily clip out parts of a complex structure, giving an unobstructed view of the structure's interior. The mixed-style presentation feature allows for a combination of display styles for different parts of molecules for pleasing visualizations of structures within structures or to highlight areas for emphasis.

Joseph M. DeSimone, *University of North Carolina at Chapel Hill*

Book Reviews

Chemistry of Solid State Materials. Volume 1. Chemical Synthesis of Advanced Ceramic Materials. By D. Segal (Harwell Laboratory, Oxfordshire). Cambridge University Press: Cambridge. 1991. xv + 182 pp. $24.95. ISBN 0-521-42418-6.

This is the first book in the new series edited by A. R. West and H. Baxter. The compact book provides a clear overview of a wide scope of ceramic materials and will be especially useful in classes on this aspect of material science as well as for a fast introduction to this field of research. The book consists of 10 chapters and one appendix. Starting with a sweep-scan of the up-to-date applications of ceramics in science and engineering, Prof. Segal guides the reader through the principal routes to ceramics and their fabrication. The book emphasizes the description of the chemical processes involved rather than discussions of chemical principles. In Chapters 4 and 5, the sol-gel processes of inorganic colloids and metal–organic compounds are described, metal–alkoxides in particular, with the latter chapter including the essential mechanisms of the hydrolysis and condensation reactions. The third chapter of "wet" routes to ceramic materials is dedicated to the less common reactions in non-aqueous media. The "solid" route to ceramics via polymer pyrolysis and hydrothermal processing of pre-ceramic powders is discussed in Chapter 7 and 8. Finally, Chapter 9 covers the reactions in the gas phase, while other miscellaneous routes of mixed nature are described in Chapter 10. In the Appendix, a most important practical aspect of ceramic materials is reviewed: determining their particle size. Supported by ca. 400 references, this book provides an efficiently highlighted introduction to the field of ceramic materials together with useful guidance for a deeper acquaintance with its specific topics. The book was first published in 1989 so that references through approximately 1987 are included. This book should be very useful as supplementary reading in any general materials chemistry class.

Y. Haruvy and S. E. Webber, *The University of Texas at Austin*

Macromolecular Syntheses. Volume 11. Editor David A. Tirrell; Editor-in-Chief Lon J. Mathias. MRG Polymer Press: Hattiesburg, MS. 1992. ix + 114 pp. $20.00 (softcover); $40.00 (hardcover). ISBN 1-881035-02-6.

This volume is different from earlier members of this well-known series only in that it has been developed using current desk-top publishing techniques to increase publication speed and reduce cost. The editors have most certainly achieved both objectives and have done it while maintaining the high standards set by the previous volumes. It is remarkable to purchase a book early in 1992 that contains references to journal articles from 1991—particularly when one considers that each synthetic procedure has been independently verified and statements from the checkers have been included.

The synthetic examples chosen for this volume cover a broad range of polymer types and polymerization procedures, making it useful to the polymer community in general. Each synthetic procedure is documented in enough detail to enable the inexperienced chemist to carry out the reaction. Areas of concern, such as hazardous chemicals or processes, are clearly highlighted. The inclusion of notes from the authors and suggestions from the checkers should be very valuable, and each article appears to be well referenced if there is any need to seek the original source. I found the articles easy to read and to follow; the editors have done a good job of both standardizing the format and eliminating errors.

As with the previous volumes, this edition provides a fast, convenient, detailed, and safe method for both polymer and nonpolymer chemists to access polymeric materials that lie beyond the scope of their expertize. It will be a valuable addition to technical and personal libraries, given that it is available in both hard- and softcover.

James M. Pearson, *Eastman Kodak Company*

Advances in Spectroscopy. Volume 19. Spectroscopy of Advanced Materials. Edited by R. J. H. Clark (University College London) and R. E. Hester (University of York). John Wiley & Sons: Chichester and New York. 1991. xix + 405 pp. $250.00. ISBN 0-471-92981-6.

This volume is comprised of six chapters, individually entitled Charge Transfer Crystals and Molecular Conductors; Non-linear Optical Spectroscopy of Conjugated Polymers; Pulsed Neutron Studies of Materials; Photoluminescence Spectroscopy of Thin Film Semiconductor Materials; Vibrational Spectroscopy of Polyconjugated Materials: Polyacetylenes and Polyenes; and Spectroscopy and Photoexcitation Spectroscopy of Polyaniline: A Model System for New Phenomena. Each chapter contains a pedagogical and largely self-contained treatment of the theoretical background of its subject and a summary of important and representative experimental findings. The chapters are uniformly carefully prepared, well written, and authoritative. The volume therefore serves as much more than a mere entry point into the literature. It should be noted, however, that the volume does not treat the spectroscopy of materials in a comprehensive way. The emphasis is on optical spectroscopy, in five of the six chapters, and on organic materials, in four of the six chapters. Thus, techniques such as magnetic resonance spectroscopy, which is of obvious importance in the characterization of the structural, dynamic, and electronic properties of materials, and materials such as ceramics and inorganic glasses, which are of obvious technological and scientific interest, are not discussed. Nonetheless, a scientist at the graduate level and beyond with an interest in acquiring a good overall knowledge of the subjects presented would certainly profit from an examination of this volume.

Robert Tycko, *AT&T Bell Laboratories*