Additions and Corrections

Cannizzaro-Based O_2-Dependent Cleavage of DNA by Quinocarcin [*J. Am. Chem. Soc.* **1992**, *114*, 733–740]. ROBERT M. WILLIAMS,* TOMASZ GLINKA, MARK E. FLANAGAN, RENEE GALLEGOS, HAZEL COFFMAN, and DEIHUA PEI

Page 736, Table I: Under entry 8 the rate constant reads 4.2×10^4. This should read 4.2×10^{-4}.

The "CUPID" Method for Calculating the Continuous Probability Distribution of Rotamers from NMR Data [*J. Am. Chem. Soc.* **1992**, *114*, 6195–6199]. ŽELJKO DŽAKULA, WILLIAM M. WESTLER, ARTHUR S. EDISON, and JOHN L. MARKLEY*

Page 6195: The last sentence of Abstract should read as follows:

The theory underlying CUPID is presented here; the accompanying article (Džakula, Ž.; Edison, A. S.; Westler, W. M.; Markley, J. L. *J. Am. Chem. Soc.*, following paper in this issue) demonstrates an application of CUPID to the analysis of experimental data for L-leucine and of simulated data for an α-helix in a protein.

Page 6198: Equation 20 should read

$$\underset{\sim}{\mathbf{E}} = \begin{bmatrix} \boxed{\underset{\sim}{\mathbf{J}}} \\ \boxed{\underset{\sim}{\mathbf{N}}} \end{bmatrix} \qquad (20)$$

Equation 25 should read

$$\underset{\approx}{\alpha} \cdot \underset{\sim}{\mathbf{U}} = \underset{\sim}{\beta} \qquad (25)$$

Equation 27 should read

$$\beta_i = \sum_{m=1}^{M_j} \mathbf{j}_m \cdot A_{mi} + \sum_{m=1}^{M_n} \mathbf{n}_m \cdot A_{mi} \qquad \text{where } i = 1, \ldots, 2N \qquad (27)$$

Analysis of χ_1 Rotamer Populations from NMR Data by the CUPID Method [*J. Am. Chem. Soc.* **1992**, *114*, 6200–6207]. ŽELJKO DŽAKULA, ARTHUR S. EDISON, WILLIAM M. WESTLER, and JOHN L. MARKLEY*

Page 6204: The sentence starting in the 11th line of Paragraph 3.2. should read as follows:

Thus the solid lines in Figures 5 and 6 show the initial distributions and the (identical) distributions reproduced by CUPID analysis of error-free data.

Computer Software Reviews

MathType Version 1.1. Design Science: 4028 Broadway, Long Beach, California 90803. List price $249.00; educational discount 25%. Upgrade for Word 2.0 owners is $89.00.

MathType is a full featured WYSIWYG mathematical equation editor that runs under Windows on IBM PC's or clones. It allows building the most complex mathematical expressions on the screen merely by selecting the appropriate elements from a pulldown menu and filling in the blanks if required. It has a symbol strip, a template strip, and a custom macro strip. It contains all the Greek symbols, integrals, matrices, summations, partial derivatives, set symbols, and every other mathematical symbol that I have ever run across. The size of delimiters such as parentheses is automatically adjusted as the size of expressions within them changes. The customizable strips allow selecting commonly used elements or expressions. The macro strip allows you to set up your most complex common expressions and select them with a single mouse click. For experienced users, all functions are called by accelerator key combinations, and you do not even have to remove your fingers from the keyboard.

MathType allows the creation of equations that can be printed directly from MathType or imported by the cut and paste feature of Windows into suitable work processor packages. In addition to generating Windows Meta Files (WMF), MathType also creates T_EX compatible ex-

pressions. For printing, MathType will work directly with many laser jet and dot matrix printers, although for the dot matrix printer you will need a font type manager.

While MathType comes with a complete tutorial, it is so intuitive that you can just dive in and be using it reasonably proficiently in 20–30 min. The manual allows you to fine tune the few less obvious things such as tabs. For example, the following demonstration expression was typeset in under 90 s.

$$\begin{pmatrix} \sum_{j=1}^{\infty} x_j^2 & \sqrt{\frac{a}{b}} \\ \alpha & \Delta \end{pmatrix} \geq \int_0^7 z^3 e^{\epsilon} \, dz = \overline{x + y}$$

The 2 × 2 matrix, the integral, the square root, the quotient, and the average all have one or more fill-in-the-blank boxes and were selected by a single mouse click. The Greek symbols were single mouse operations from the symbol template.

As supplied, MathType uses the standard typesetting rules for equations. The average user will be satisfied by the defaults. However, everything is adjustable by the user including fonts, sizes, and spacing. Fine tuning can be performed by moving any component by single screen pixels at 100% viewing. Higher resolution is provided by the expanded views (one quarter pixel at 400%).

Anyone familiar with the equation setter in Microsoft Word 2.0 for Windows has already used a subset of MathType. The Word version condenses more functions into pulldown menus, which slows use by requiring subselection of items, lacks user configurable popups, templates and macros, and does not have all the flexible formatting features of MathType. While the Word version is good for small equation setting problems, serious setters will find the full MathType version indispensable.

As far as using MathType for setting equations, it worked flawlessly and is a true pleasure to use. However, there were problems. It is supposed to work directly with an HP LaserJet II with extra memory but no font cartridges (it can exploit font cartridges if available). Even with extensive and very helpful assistance from a Design Science technical support engineer, we were never able to get it to print properly; the MathType fonts were not being successfully downloaded. When I received Word, which had the necessary True Type scalable fonts, the problem went away. The True Type fonts were successfully downloaded as predicted by the engineer. According to Design Science, the True Type scientific fonts will be included in the upcoming release 3 (there will be no release 2) but are not included in the current version. On the other hand, MathType worked flawlessly under Windows 3 or 3.1 with a PostScript printer.

There are problems with the transfer of equations from MathType to other word processors. The latest release of WordPerfect 5.1 for Windows (4/30/92) accepts cut and paste from MathType only if you are using the Windows print drivers; you cannot have a WordPerfect print driver installed or both the screen and printout are trashed. The WordPerfect people are working on this problem. For Word, which uses a subset of MathType, you would have expected few or no problems. However, there are difficulties. While you can cut and paste expressions into Word, any attempt to edit them with Word immediately trashes the expression. Word does not recognize the MathType format, believes it to be a drawing, and messes it up when it tries to load the equation into the drawing editor. The error is irreversible unless you have kept a separate copy of the equation. You can also paste the equation into the Word equation editor, but this can result in some loss of formatting flexibility. Version 3 will solve this problem by including OLE (object linking and embedding).

In summary, MathType is an outstanding tool to those who have to set modest to complex scientific equations. For those who have had to set equations using the UNIX eqn or the WordPerfect 5.1 variant, one taste of MathType and you will never go back. When the file format problems are overcome, it is difficult to envision a more perfect product.

*Book Reviews**

Physical Sciences Data. Volume 43. Vapor–Liquid Equilibrium Data—Salt Effect. By Shuzo Ohe (Science University of Tokyo). Elsevier Kodansha: Amsterdam-Tokyo. 1991. xxxii + 360 pp. $218.00. ISBN 0-444-98687-1.

This monograph has been centrally concerned with the topic of reducing distillation problems involving separations of azeotropic mixtures by taking advantage of the salt effect disturbance of the ratios of solute and solvent in the vapor and liquid phases. Such salt effect disturbances seem generally to have been less widely exploited in commercial processes than disturbances effected by additions of volatile components. This has been importantly related to a lack of accurate theoretical predictions of the effects of additions of particular salts to different solute/solvent systems.

The main content of the monograph comprises some 700 illustrative plots of parameters related to vapor–liquid equilibria for a very comprehensive collection of solute–solvent systems. A preceding guide sheet to the component features of diagrams is provided. In general, the plots seem favorably to compare experimental findings of alterations of the parameters produced by a variety of different salts and their concentrations with predicted relationships calculated from considerations of the preferential solvation approach developed by the author.

The data sheets are preceded by an introductory preface and some 20 pages of introductory and explanatory referenced text. Unfortunately this section has been rather poorly edited, which has resulted in it being somewhat difficult to make easy correlations with the tables and figures contained throughout the text.

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Perspectives of Nonlinear Dynamics. Volumes 1 and 2. By E. Atlee Jackson (University of Illinois). Cambridge University Press: Cambridge. 1991. Volume 1: xix + 496 pp. Volume 2: xvii + 633 pp. Volumes 1 and 2: $69.95 (hardback) and $32.95 (paperback). ISBN 0-521-34504-9 (Volume 1, hardback), 0-521-42632-4 (Volume 1, paperback), 0-521-35458-7 (Volume 2, hardback), and 0-521-42633-2 (Volume 2, paperback).

Nonlinear dynamics occupies a peculiar place in chemical research today. Its importance, in such fields as combustion, spectroscopy, and chemical oscillations, is growing rapidly, yet almost none of its practitioners received any formal training in the subject, and there are few courses on nonlinear dynamics being taught in universities at a mathematical level accessible to most graduate students in physical chemistry or chemical physics.

This two-volume set may provide at least a partial remedy for this gap. These books represent an attempt to "afford an introductory access to concepts which will stimulate imagination in the future". Jackson identifies these concepts as (1) classic and modern analytic methods, (2) topological and other global viewpoints, and (3) computational and heuristic approaches. The first two areas are treated more thoroughly and more satisfactorily than the third, but since most students of chemistry find numerical techniques easier to grasp than "purer" mathematical ones, the weakness in the numerical area is not a fatal one.

Jackson's treatment is somewhat idiosyncratic. The book was clearly written by an interesting person who is fond of his subject matter. The cartoons and occasional digressions (e.g., on the wisdom of attempting to apply catastrophe theory to social problems) make the books more entertaining, though they do contribute to their length. Jackson places great emphasis on intuition and thoughtful approximation, characterizing as "myths" the commonly held notions that linear equations are easier to solve than nonlinear equations and that an analytical solution, if it exists, gives the most useful information about a system. One of the strongest points in Jackson's treatment is the inclusion of many cleverly constructed exercises, supplemented by very helpful "comments" that range from complete solutions to encouragement to struggle on. The historical perspective Jackson presents is another attractive feature, as is the 6-page glossary of mathematical terms and symbols.

The focus is on ordinary differential equations and difference equations (maps), especially with a few degrees of freedom, and these are treated in considerable detail. Partial differential equations and cellular

*Unsigned book reviews are by the Book Review Editor.