

## Additions and Corrections

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**Table of Marks and Double Cosets in Isomer Counting** [*J. Am. Chem. Soc.* **1987**, *109*, 2130–2137]. C. ALDEN MEAD

Page 2136, Table XV: The entry in the lower right-hand corner of this table (row and column  $C_1$ ) should be  $1/4$ , not  $1/2$  as shown. This does not affect any of the results of the paper.

The author is grateful to P. Deck and S. Jons for calling this error to his attention.

**Magnetic and Spectroscopic Characterization of an Iron Porphyrin Peroxide Complex. Peroxoferrioxoethylporphyrin(1-)** [*J. Am. Chem. Soc.* **1988**, *110*, 1382–1388]. JUDITH N. BURSTYN, JAMES A. ROE, ANDREW R. MIKSZTAL, BEN A. SHAEVITZ, GEORGE LANG, and JOAN SELVERSTONE VALENTINE\*

Page 1386: Figure 7A should be identified as 7B, and vice versa.

**Transition Structures of Aldol Reactions** [*J. Am. Chem. Soc.* **1988**, *110*, 3684–3686]. YI LI, MICHAEL N. PADDON-ROW, and K. N. HOUK\*

Page 3685: The column heads for the second and third columns from the right in Table I labeling attack angles on the carbonyl and the enolate are reversed.

## Computer Software Reviews

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**WormStat.** Small Business Computers of New England, Inc.: P.O. Box 397, 4 Limbo Lane, Amherst, NH 03031. List price \$19.95; site licence \$600.00.

Wormstat is a statistical package for use on Macintosh computers. It is extremely user friendly having been designed with a "Macpaint" like format. There are 16 statistical tools on a "Macpaint" like palette and by simply clicking the appropriate tool various analyses can be carried out. Data can be entered from the keyboard by opening a data file or by transfer from another application with Copy and Paste. There are two versions—one for a 128K Macintosh and one for a 512K or larger Mac. On the program for a system with smaller memory, the data can be entered into a data matrix of 10 columns of 200 numbers each. With the program for a larger system, a maximum of 600 numbers can be entered into each of 10 columns, although the directions indicate 1000 numbers are possible. Various features such as addition, multiplication, square root,  $z$  score, etc., are available for transforming data that are already in a column, and up to 600 numbers can be generated in a given column from a normal or uniform distribution. The columns can also be filled with zeros or sequential integers.

The palette is quite easy to use, but in most cases it only works for one column at a time. Thus, as one clicks through the items—mean, medium, standard deviation, and range—each value is added to a box on the screen one at a time. In order to get the statistics for another column of data, the above procedure must be repeated again, which is a slow process. Other tools that are available are histogram plot, box and whisker plot,  $t$  test,  $F$  test, one way analysis of variance, chi square test of independence, Mann Whitney  $U$  test, Wilcoxon test, scatterplot, correlation moment, and linear regression line and coefficients. The histogram is not very informative since the abscissa is in units of  $\pm 1$  standard deviation. A nice feature of the program is the availability of a probability menu which has normal,  $t$ ,  $F$ , chi square, and binomial entries. For a given statistic and the degrees of freedom, a probability curve can be shown graphically and an exact probability calculated.

A poorly designed feature of the program is that a biased number of degrees of freedom can be used. Also, the linear regression analysis does not give the standard error of the intercept and slope nor does it give residuals. This program has some very nice pedagogical features like probability curves with areas corresponding to the obtained value shaded

in, and a hand drawn regression line for comparison to the actual regression line. On the other hand, certain features found in more research oriented statistical packages such as multiple regression and two way analysis of variance are missing. Overall, the program best serves as a method for doing simple statistical tests or as a teaching tool for introducing some introductory concepts in statistics.

R. L. Blrke, *City College, New York*

**ChemDraw. Version 2.0.** Cambridge Scientific Computing: 875 Massachusetts Avenue, Suite 41, Cambridge, MA 02139. (617) 491-6862. List price \$595.00; academic discount \$396.00; student license available. Not copy protected.

ChemDraw is a drawing program for generating publication-quality chemical structures and figures on an Apple Macintosh Plus, SE, or II microcomputer. The program provides tools for the drawing of complex organic molecules and reaction schemes. A variety of other tools allow the addition of captions, special figures, and other features.

When the ChemDraw program is first run, the user is presented with a blank page and a "palette" of drawing tools. The tools include several types of bonds, such as line, wedge, and dash; several types of rings, such as saturated or unsaturated five-, six-, seven-, or eight-membered rings; text tools for adding captions and for changing atom labels; several types of parentheses and brackets; shaded depictions of common atomic orbital shapes; several arrow tools, such as reaction arrows, equilibrium arrows, retrosynthetic arrows, and arrows depicting flow of electrons; and a lasso and eraser tool for modifying structures on the screen.

Drawing a chemical structure in ChemDraw is a simple matter of choosing the appropriate tool, such as a bond tool or a ring tool, and clicking the mouse on a clean part of the work page. Structures can be built up easily with the available tools or modified from structures already drawn in ChemDraw and saved previously. Once a structure is drawn, say on the left side of a reaction arrow, it can be copied to the right side of the equation and modified. The ability to copy and modify structures lends a consistency of style to a document prepared with ChemDraw.

Captions, titles, and other text are easily added with the text tool. The text tool allows captions to be written by using any combination of styles, such as italics, boldface, super- and subscripts, underlining, and so on.