Additions and Corrections

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. Peroxoferrioctaethylporphyrin(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

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, Wilcoxin test, scatterplot, correlation moment, and linear regression line and coefficients. The histogram is not very informative since the abscissa is in units of ±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 grapically 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.

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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.

The full set of fonts installed on the Macintosh are available from within ChemDraw.

A number of customizable options can be set and saved in a "preferences" file. These settings are recalled whenever the program is run. Included among the settings is an option for bonds and rings to be drawn in a pre-specified size (fixed length), an option to display guides for laying out 35 mm slides on the page, and options for default caption and atom label styles.

Once chemical structures or reaction schemes are drawn in ChemDraw, they can be arranged on the page with the Show Page option. This option gives a miniature view of the entire page, allowing the user to shift portions of the drawing on the page for a more pleasing layout. The page can then be printed on either an Imagewriter dot matrix printer or a LaserWriter laser printer. Alternatively, structures can be exported into other documents, such as word processor documents, by use of the Macintosh clipboard.

ChemDraw documents can also be used as input files for the Chem3D program.[1] This capability allows for easy setup of chemical structures for three-dimensional manipulation.

ChemDraw is a full-featured, easy-to-use drawing program for generating chemical reaction schemes and structural formulas. It is intuitive to use and adheres well to the standard Macintosh user interface. The printed output is equal or superior in quality to pen-and-ink drawings, especially when printed on the Apple LaserWriter printer. The ability to copy and modify structural formulas lends consistency of appearance to drawings; the inclusion of a Preferences file maintains consistency between documents. This program will be a useful addition to the software library of any chemist who publishes structural formulas and reaction schemes.

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(1) Following review in this journal.

Chem3D. Version 1.0. Cambridge Scientific Computing, Inc.: 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.

Chem3D is a molecular modelling computer program that could replace the chemist's traditional plastic model kit. The program runs on an Apple Macintosh Plus, SE, or II running System upgrade 5.0 or higher. Chem3D provides powerful yet easy-to-use tools for the construction and manipulation of complicated molecular structures in three dimensions. Any geometrical measurement from the structure is readily available merely by selecting the atoms or bonds to be measured with the mouse. Structures can be rotated, resized, and even animated for better visualization of geometrical relationships between atoms and groups.

A chemical structure can be built with the Chem3D program itself or it can be imported as a ChemDraw[1] file or as a coordinate file. An sp^3 carbon atom serves as the default starting point for new molecules built within the Chem3D program, though the default can be set to any other atom type by the user. Molecular structures may be built up by adding atoms or substructures or by modifying atoms in the existing structure. Any atom in the periodic table can be accommodated, with geometries including trigonal bipyramidal, octahedral, and irregular geometries of up to ten ligands. The structure can be refined by eye by translating atoms or rotating groups in three dimensions with the mouse.

For building complicated structures from scratch, it is usually easier to import them as two-dimensional ChemDraw files. Chem3D reads ChemDraw files directly, converting them to three-dimensional representations with standard bond lengths and angles from the Chem3D parameter file. Chem3D correctly interprets stereochemical designations such as dashed or wedge bonds or H-dot notation in fused rings.

Chem3D can also read Cartesian or crystallographic coordinate files. However, additional information must be added to these files in order to read them into Chem3D structures. Each atomic type must be designated by a "text number", which may be found in an appendix in the program documentation. A different text number is assigned to every atom type. For example, an sp^2 carbon atom is assigned text number 63, while an sp^3 carbon is assigned 64. Also, the coordinate file must list all the bonds between atoms. The inclusion of this extra information in the input file is somewhat laborious and time-consuming.

Powerful tools are available for manipulation of molecular models once they are entered into the Chem3D program. Any bond length, bond angle, or dihedral angle can be manipulated either by eye, using the mouse, or by entering a numerical value. The structure can be rotated about three orthogonal axes. Groups of atoms can be selected and rotated with respect to the rest of the model. All manipulations are stored as "views" up to the memory capacity of the computer on which the program is running. All prior views retain their geometrical information, so that a "multiple undoing" of manipulations is possible. The manipulations can be animated, replaying through all the views in memory. This feature is convenient for displaying a slowly rotating model on the screen.

After the model has been refined and suitable views have been chosen, the picture can be printed out on either a LaserWriter or Imagewriter printer. Interestingly, files printed on the LaserWriter are downloaded to the printer in a few minutes, but they may take 15–20 min to print. The structure can also be written to disk as a Chem3D file, a ChemDraw file, an internal coordinate file, or a Cartesian coordinate file.

Chem3D provides many options for construction and manipulation of molecular models. However, the program does suffer from several shortcomings. The ability to replace atoms with substructures loses some utility because so few substructures are included with the program. Eight hydrocarbon substructures are included in the Chem3D parameter set and 29 substructures are included in the MM2 parameter set. The hydrocarbon residues are redundant, since they can be built readily within the Chem3D program with standard bond angles and lengths. Of the 29 structures included with the MM2 parameter set, 18 are amino acids. The remaining structures include carboxyl, amide, and ester functional groups and a couple of saturated hydrocarbon residues. The user can augment the library by adding frequently used moieties after building them by one of the methods described above.

The program currently does not support color or gray scales on the Macintosh II, though support of color would greatly enhance the quality of pictures obtainable. If color were supported, lecture quality slides could be photographed from the video display itself. The program seemed to have several problems updating the display, particularly when windows were moved on the screen. Chem3D does not generate space-filling ("CPK") representations, although the radii of the atoms in the display can be adjusted up to the van der Waal's radius of the atoms.[2]

It would be nice if future versions of the program offered the enhancements mentioned above, as well as several others. Chem3D could offer interfaces to commonly used computational programs such as MM2, Gaussian 8X, and MOPAC. Such an interface could consist simply of an option to save structure files in a format suitable for input to these programs. The program could also be extended to offer simple calculations on the Macintosh itself. Currently, the program can optimize dihedral angles of ring closures; however, the structures that result from optimization often have unrealistic bond lengths and angles.

Chem3D has much promise as a three-dimensional molecular modelling program for the Macintosh. It offers flexibility in building and displaying molecular structures. Geometrical relationships in a molecular system may be appreciated, perhaps leading to new insights.

David S. Allan, *University of Michigan*

(1) Chemical structure drafting program for publication quality drawings, available from Cambridge Scientific Computing, Inc.

(2) Features slated for version 1.1 will correct many of these shortcomings.