heterocumulene. Alternatively, SO_2 could initially coordinate to the sulfur atom of -SH, similar to $RS-SO_2$ in $L_nCuSR\cdot SO_2$.[14] In both cases, base-assisted proton transfer to an oxygen atom could result in formation of an $MSSO_2H$ group. Since the SO_2H unit is unstable in both RSO_2H[15] and novel MSO_2H complexes,[2c] the proposed $MSSO_2H$ group would likewise be expected to decompose to reduced sulfur species, such as **3**, and H_2O. The implications of this chemistry could extend to heterogeneous sulfide

catalysts such as hydrodesulfurization catalysts[16] and we plan to investigate these catalysts for SO_2 reduction.

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(17) SO_2 amounts were measured on a vacuum line by using $P-V-T$ data. After the reaction mixture was quenched (−196 °C) and H_2 pumped off, unreacted SO_2 was isolated by pumping (25 °C) and passage through a −95 °C trap.

Computer Software Reviews *

MacDraw. By Mark Cutter. Apple Computer, Inc.: Cupertino, CA. List price $195.00.

MACDRAW is a graphic design program for use in creating pictorial layouts that involve relatively fixed, uniform objects. MACDRAW is a release of Apple Corporation and will operate only on the MacIntosh computer. The disk operating system is the standard MacIntosh Finder and the current release, 1.7, is non-copy protected. MACDRAW will operate on either a 128K or 512K MacIntosh although it was evaluated for this review on a machine with the larger memory capacity.

MACDRAW is an object oriented drawing program and as such differs from the more well known MACPAINT as the latter maniuplates and stores information in screen pictal point format. Thus, the basic underlying principle of these two programs is entirely different and each has its strengths and weaknesses. However, for use in creating scientific layouts such as chemical structures, MACDRAW is superior. MACDRAW has a standard set of drawing tools that allow the creation of such objects as lines, circles, ovals, squares, rectangles, and odd-shaped polygons with an unlimited number of corners. In addition, there is the capability of drawing arcs and random lines. When an object, such as a square, is created, certain defaults are automatically assigned to the object such as the line width and the fill. These defaults may be changed and there are four different line thicknesses as well as the opportunity to create an object with no border line. There are as well a whole series of fill patterns that can be used. All of the characteristics of an object can be modified.

As each object is created, it is not only placed on the diagram in an X–Y coordinate sense but also it is stacked in front of all previous objects. This has the result that objects with fill will cover those which were created first. This stacking order is not permanent and can be changed by selecting objects and either moving them to the front or moving them to the back of the stack. This is an extremely useful feature because it allows the creation of small shapes with the fill white but no lines. Placing such an object between two polygons whose lines cross creates the sense of three-dimensionality since the line of the back polygon will be broken. This has the interesting feature that simply by reordering the stacking position the objects can be switched from one mirror image sense to the other. Once objects are created they may be moved, duplicated, flipped along either the vertical or horizontal axis, and rotated by 90° increments. They may also be resized, and with the option of showing size active the dimensions of any object will be displayed on the screen. In addition, when the show size option is activated the dimensions of objects are displayed as they are created. Thus, the length of a line is dynamically displayed as it is formed and it is quite easy to obtain precise lengths. For squares, rectangles, circles, and ovoids, the two pertinent dimensions are displayed while for polygons the rise and run number from the last point is illustrated. This feature makes it quite simple to create regular patterns such as hexagons or the normal zigzag of an acyclic carbon chain based on simple trigonometric calculations. Not every line length and rise and run is available, however, as MACDRAW will allow no greater precision than the pictal display on the screen. One can operate either in an English or metric system and in both cases the actual size on the screen is quite close to the printed version. In the metric mode, one can access dimensions that vary by approximately 0.03 cm. This would appear to be more than sufficiently precise for routine structure drawing purposes.

There are three views which can be accessed of any document that is currently active: the normal view which, as indicated above, has nearly

the same scale as the printed version; an intermediate view; and a reduced to fit mode that displays the entire document. The document can be adjusted to print on anywhere from one 8.5 × 11 in. sheet to a maximum of 5 × 12 such sheets which can then be pasted together to make an extremely large layout.

The reviewer found it convenient to work with structures that had a uniform 2 cm bond length. A template was created with common structural subunits such as hexagons, pentagons, etc., and these were quite easy to create with nearly exact dimensions. Up to four documents can be kept active on the desktop at one time, and thus the template can be kept accessible. Objects can be copied from the template to the clipboard and then pasted into the drawing being created. After objects are pasted into the active document they may be moved with facility and the lines of two adjacent objects such as two hexagons can be made to merge.

A collection of objects such as that which would represent the steroid nucleus can then be grouped together in which case MACDRAW treats them as a single object. They can then be duplicated, placed in various positions around the diagram, and further manipulated by the addition of structural subunits that vary from one to another. A very useful feature of MACDRAW is that when an object is duplicated and then moved in the diagram a repeat of the duplication object will result in a second copy being placed at the same displacement from the first duplicate as the first duplicate was from the original. This permits very ready setup of repetitive layouts, for instance in synthetic schemes where the basic structure stays unchanged and functional manipulations are being carried out. Thus, for instance, a single steroid nucleus could be placed in the upper left hand corner of a document, duplicated, the duplicate placed on the same line but in the middle, duplicated again to create a third all of which are evenly spaced across the top of the document. These three then can be duplicated together and if that set of duplicates is moved to the middle of the sheet and duplicated again one will arrive at nine identical units placed uniformly on the document. MACDRAW has the feature of showing rulers along the left and top margin which indicate the position on the page. While this can be used to align objects, the reviewer found it easier simply to create temporary vertical and horizontal lines as an alignment grid. Once objects were appropriately positioned, these temporary lines were removed.

Text may be created in two modes, a caption and a paragraph display. The former is useful for short text entries such as structure numbers and information that would typically go about a transformation arrow while the latter contains the feature of work wraparound and is useful in creating fairly extensive amounts of text. Text, like other objects, can have fill and for creating structure diagrams the most useful fill is white where a single letter such as an "N" or an "O" will cover up structure lines that are on objects behind the letter. Text within the caption mode can also either be left, centered, or right justified and for the purpose of adding heteroatoms to structures the center mode is to be preferred since then the fill cover is then symmectrical about the letter.

Printing MACDRAW diagrams can be accomplished either with the Apple Imagewriter or with the Apple Laserwriter. The former has the option of printing either full scale or in a 50% reduce mode where the latter reduces both dimensions by half, resulting in a final printed area of $^1/_4$ of the original as it was operated on under MACDRAW. With 2-cm bonds the dimensions then are reduced to 1 cm, which are slightly too large for final printed versions. However, these may be reduced during the publication process to whatever is appropriate for a particular journal or the originals may be reduced by using photocopiers of the Xerox type

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which have reducing capabilities. The Laserwriter options are more powerful, and any incremental reduction from 100% down to 25% can be used. The Imagewriter in 50% reduction mode results in quite acceptable images (Figure 1) while the Laserwriter when used with the smoothing option results in pictures which are fully the equal of hand done, line drawings (Figure 2).
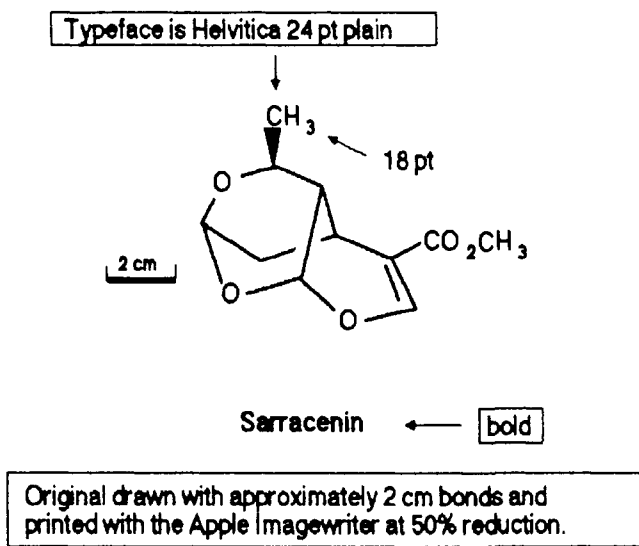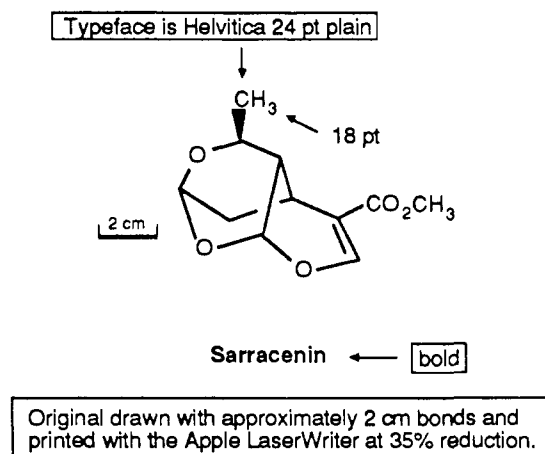

Figure 1

Figure 2

Both an excellent manual as well as a tutorial tape are provided, and while those experienced with other MacIntosh software will be able to use MACDRAW without consulting either, a complete reading of the manual is highly recommended.

Overall, MACDRAW is an extremely powerful drafting tool which fits very well into the needs of the chemists to create structures. It has nearly the full range of capabilities that would be desired, and this reviewer noted only the lack of the ability to rotate objects to a finer degree than the 90° offered. However, although this may appear to be a significant limitation, only a relatively small amount of additional effort needs to be expended in creating the master template to overcome this drawback. The reviewer has extensive experience in creating line drawings using rapidiographs, chemical templates, and transfer letters but found that with only two or three hours of experience with MACDRAW that single structures could be created in approximately $^1/_2$ the time using MACDRAW. The facility with which structural subunits can be duplicated and with which textual information can be entered makes for an even more dramatic time saving.

While the full range of MacIntosh fonts are available, the reviewer would recommend the adoption of the Helvetica font for chemical purposes as it is the cleanest of the fonts that are stored internally in the Laserwriter. While it is tempting to use the Princeton font because of its super- and subscript capability, this font and, as well, any of the MacIntosh which is not internally stored in the Laserwriter lengthens the printing process dramatically.

BALANCE. By D. L. Massart, M. P. Derde, Y. Michotte, and L. Kaufman. Elsevier Scientific Software: 52 Vanderbilt Avenue, New York, NY 10017. 1984. List Price $150.

This program is designed to carry out statistical tests on two sets of measurements to determine whether the two series can be considered to give different results, i.e., whether the means are significantly different. It could be used to compare results from two analytical methods, two sets of clinical data, etc. It incorporates the following tests: tests for small numbers and for large numbers of observations; independent and related (paired) tests; one- and two-tailed (sided) tests; Student's and Cochran's tests (parametric tests); Wilcoxon's matched-pairs signed-rank test and Mann-Whitney's U-test (nonparametric tests).

The two data sets to be compared can be entered from the keyboard or from sequential text files on disk. Since the structure of the disk files is described in the documentation, this latter option would make it convenient, for example, to use data sets gathered under computer control and written to disk by the experiment program. An easy-to-use editing feature allows reviewing, modification, and saving of data sets.

The program is quite easy to use, prompting liberally for one-keystroke responses to select options. The documentation is among the best this reviewer has seen. An especially useful section provides a short course in statistical testing. Here the user who may be somewhat unfamiliar with statistical jargon can learn without derivations or other distractions about the distinctions among the various statistical scales (nominal, ordinal, interval, and ratio), the differences between parametric and nonparametric tests and when each would be suitable, the distinction between related (paired) and independent samples and the test appropriate for each sample type, and the necessary statistical jargon regarding the null hypothesis, level of significance, one- vs. two-sided tests, confidence level, etc. The authors are especially careful to explain the approach and criteria used in each type of testing method and to warn the user about the conditions for applicability of each type of test—e.g., suitability for large (>30) or small data sets or dependence on normality of distribution and on equivalence of variances of the two groups (using the Fisher-Snedecor F-test). Even more usefully, the program is constructed to automatically determine which tests are suitable for the data at hand and to guide the user to the most appropriate tests and avoid inappropriate ones. Frequent use of worked numerical examples in the manual makes this an excellent review of basic statistical testing procedures.

The documentation package also includes a complete listing of the BASIC source code. This is liberally annotated with REM statements, making it easy for the knowledgeable user to adapt the program to specialized applications. A thorough flow diagram of the program is provided.

The program as supplied and reviewed is operational on the Apple II, II+, and IIe microcomputers, running in the APPLESOFT BASIC language with the DOS 3.3 operating system. Running on the standard 48K machine, the program as written accommodates up to 100 values in each of the two groups of data, with instructions on re-dimensioning for larger cases. It can be operated with one or two disk drives and with or without a printer. The program is supplied on a write-protected disk with instructions for copying to a user disk (using standard copy procedures) before initializing this user program disk to the particular hardware configuration. This approach thus provides unlimited backup protection. The disk includes a compressed working version of the program (in BASIC, not very legible but efficient in execution) and a fully documented version, corresponding to the source listing in the manual and suitable for study or modification. The User Guide section of the manual includes numerical examples to exemplify use of the program. A version for the IBM-PC is also available at the same price.

Though the manipulations carried out are standard statistical techniques, the BALANCE program and its documentation are so clearly written that it should be quite useful in many areas of academic and industrial chemistry.

Raymond E. Davis, *The University of Texas at Austin*

DIGITAL PAINTBRUSH. The Computer Colorworks, A Division of Jandel Corporation: 3030 Bridgeway, Sausalito, CA 94965. List Price (including hardware) $450.

The DIGITAL PAINTBRUSH is a desktop unit which, with its accompanying software, functions like a tablet or mouse to carry out a wide range of functions, including the following: graphics creation—elastic lines, rectangles, circles, bar-graphs, pie-charts, automatic 3-D, multiple-point curve fitting, pick-up, move, enlarge, contract. A library of symbols and images is available. Text in various fonts can be added

to any of the graphics. Scientific programs include planimetry, with the area calculated in any units; distance calculations of straight or curved lines; point by point digitizing; and basic statistical calculations. Engineering, architecture, and construction applications include basic elementary CAD-CAM with "magnetic" grids for layouts and instant, aligned separations for area or volume measurements. Print-out works with all popular dot-matrix printers and with selected color printers. Print-out size and placement can be regulated when printing graphics.

The hardware/software package is available for Apple II+, IIe, and IIc and for IBM-PC, XT, and AT and compatibles using DOS 2.0 and higher. It may be used with single or double disk drives, but it will accommodate up to 26 disk drives; 256K of memory is required for the IBM. A color-graphics adapter and a game control are required for installation. There is no copy protection and as many copies as needed for back-up may be prepared.

The DIGITAL PAINTBRUSH hardware consists of two elements: (1) a ball point pen-like stylus that is the input device for all functions (cursor/drawing control and menu selection and control) and which allows for natural, one-handed pen-on-paper operation, and (2) two rotating potentiometers housed in a durable plastic case and attached to the pen tip by strong lightweight control lines. Movement of the pen is detected by the potentiometers and interpreted by the system software to place fast and accurate reproduction of pen movements on the computer screen.

The software is extremely easy to learn and use. The manual is well-organized and written, but the operations can often be carried out with little or no recourse to the manual. The software does what it is designed to do and it can readily be adapted to other uses. For example, although a chemistry template is provided with some cyclic skeletal structures, custom design of organic molecular structures and reproduction of spectrograms of infrared and nuclear magnetic resonance is easily done. Individual sections of a document can be saved to disk and recalled for use in other layouts. Designs can be edited after they are formed, by movement about the layout and by pictal point modification of a highly magnified view. Characters can be added to structures, but hiding of lines must be done by erasing portions at the pictal level. Hard copies can be obtained using a dot-matrix printer.
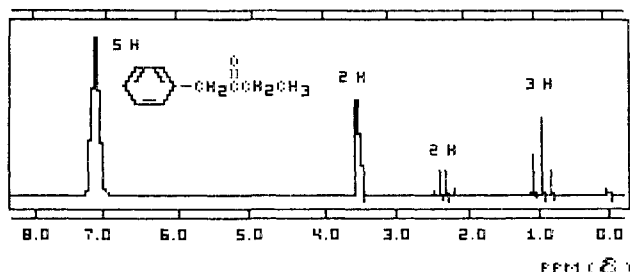
A presentation program enables users to store, organize, and display pictures in the form of a slide show. Color slides can be created from the display screen with extra equipment.

The price of the hardware/software package is $299 for the Apples

and $450 for the IBMs, plus $4.50 shipping and handling charges. The supplier does not recommend the Apple version for detailed, scientific purposes.

Royston M. Roberts and Ted S. Wen, *The University of Texas at Austin*

INSTRUMENTUNE UP. By S. N. Deming and S. L. Morgan. Elsevier Scientific Software: 52 Vanderbilt Avenue, New York, NY 10017. 1984. List Price $150.

This software package enables the optimization of up to ten variables which might impact on the performance of an instrument. A simplex optimization method serves as the base by which the program operates. There is no provision for automatically having the program tune the instrument (i.e., no A/D or DAC I/O provisions). While the title and documentation suggest instrument optimization, the program will work for optimizing any multiple parameter problem.

The program is available in Applesoft for Apple II, II+, and IIe equipped with DOS 3.3 and at least 48K RAM, as well as in PC-BASIC for IBM-PC and IBM-XT (64K RAM version) with PC-DOS 2.0. Further implementations may be developed. The publisher should be contacted for more information. A minimum of one disk drive is required and little is gained with multiple drives. Options exist for obtaining hard copy, but a printer is not mandatory for operation. The original disk is write protected, but the disks are directly copyable and backup copies are easily obtained.

The simplex technique is one of the more commonly used methods for optimization, and both authors have considerable, published experience with it. The software has no flashy graphics or exotic displays; only simple text requests for input and results of progress are presented. It employs a double-check approach ("Is this OK?") to correct for miskeying should the "enter" or "return" key be hit before the error is noticed. The disk comes with two BASIC versions of the program (documented and undocumented) and a tutorial, which carries the user through a practice run (although the manual is sufficiently complete that the tutorial is not essential). The program logic is easy to follow with the documented version should changes or modifications of the software be desired. A listing of the documented version is also included in the manual. The manual is complete and includes well-written instructions on the running of the software as well as the technical background for the simplex method.

Options are available for either "fixed size" or "variable size" simplex algorithms. Simplex edges can either be tilted or parallel to the parameter axes, and a maximum or minimum instrument response can be selected for optimization. Verification that the located optimal conditions represent the global optimum and not a local optimum is not done automatically. However, the manual addresses this issue and what can be done to check the outcome. Computation time is sufficiently short that the user will not feel that he is "waiting for the computer".

In general, this "no frills" software package could be easily and successfully used by anyone with a desire for instrumentation optimization. While sufficient documentation exists in the literature for constructing such a program, the time investment in software development must be weighed against the $150 price tag for this product. To the best of this reviewer's knowledge, no "public domain freeware" exists to duplicate this package, although it is highly probable that a large number of similar programs developed in-house exist within the scientific community.

James A. Holcombe, *The University of Texas at Austin*