

sidebands become progressively more intense. In order to achieve close agreement with the experimental MASSLF pattern the chemical shift anisotropy (CSA) must be included. At the relatively low field strength used here (2.35 T), the principal effect of the CSA is to introduce asymmetry about the centerband as shown on the right of Figure 2. Fortunately the full CSA tensor need not be precisely known. For the 2-MTHF methine many essentially identical fits can be found as long as the span of the CSA is approximately 3200 Hz, and the C-H vector is within 35° of perpendicular to the most high field tensor component. The extremely good fit of the experimental biradical MASSLF pattern in Figure 1B was the result of dozens of simulations. These calculations indicate that the difference between the highest field and lowest field CSA components can be no more than 3000 Hz (119 ppm) and no less than 2000 Hz (79 ppm). The best fits with the larger CSA require an r_{CH} of 1.08 Å; for the smaller CSA an r_{CH} of 1.07 Å provides the best agreement. The variation in the MASSLF pattern as the H-C-H angle is opened up for the larger CSA is shown to the right of Figure 2. In all of the cases investigated the H-C-H angle is required to be close to 120°. No reasonable fits can be found once θ becomes larger than 122.5° or smaller than 115° as judged on the basis of the sum of the squares of the deviations in sideband intensities.

The absence of a contact shift in either **1a** or **1b** rules out a triplet ground state for both as argued previously.¹ This fact, in conjunction with the determination of the H-C-H angle in **1a** as 120° and the observation of a CSA half that found in alkenes, provides compelling evidence for the formulation of both species as singlet biradicals.

It should be noted that an effective homonuclear decoupling scaling factor has been determined by fitting the experimental

patterns for the 2-MTHF glass assuming that all the C-H distances are 1.09 Å. Other workers⁴ have shown that this approach largely corrects for motional averaging by high frequency vibrations and lattice motions. The C-H distances so derived are then relative to the choice of r_{CH} for the 2-MTHF centers. Large amplitude motions are probably not important here as even the rotation of the 2-MTHF methyl group is slowed sufficiently to display dipolar couplings at 77 K. The sidebands in this MASSLF pattern are not resolved, which indicates that the methyl rotation rate is on the order of the dipolar couplings or the MAS spin rate. This is consistent with the value of 3.6 kcal mol⁻¹ reported¹² for this barrier. The barrier to rotation for the methylenes in **1a** must be somewhat higher than this as their MASSLF pattern shows no indications of such motional averaging.

In conclusion it has been demonstrated that 2D MASSLF methods in combination with matrix isolation NMR techniques can be used to accurately measure bond lengths and bond angles in captive intermediates. The method also provides for spectroscopic assignment of ¹³C CPMAS matrix isolation spectra. Use of higher field strengths and lower temperatures in principle should extend the method to natural abundance samples and to species isolated in rare gas matrices.

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(12) Durig, J. R.; Kizer, K. L.; Karriker, J. M. *J. Raman Spectrosc.* **1973**, *1*, 17-45.

Computer Software Reviews

SlideWrite Plus. Version 2.1. Advanced Graphics Software Inc.: 333 West Maude Avenue, No. 105, Sunnyvale, CA 94086. (408) 749-8620. List price: SlideWrite Plus 2.1 \$345.00, Fonts & Figures, \$99.00.

SlideWrite Plus is a graphics software package for any 100% IBM compatible personal computer from the PC to the PS/2. This package enables one to create assorted types of graphs (bar, pie, line, scatter) and augment them with curve fits (linear, exponential, polynomial, and others), textual annotations, and clip-art figures. As the name suggests, SlideWrite files can be used to produce slides using the HP 7510, the ImageMaker, or the Polaroid Palette Plus. It also will produce NAPLPS files (with certain size limitations) for use with General Parametrics VideoShow, ColorMetric board, and PhotoMetric camera. To run SlideWrite Plus one must have at least 390 KB of free memory, 2 disk drives or a hard disk, DOS 2.0 (or later), a graphics adapter (AT&T 6300, Hercules Graphics Card, IBM 3270 APA Card, IBM Color/Graphics, EGA, or VGA), and the appropriate monitor. In addition it is very useful to have a mouse. The output can be sent to the screen, a dot matrix or laser printer (1 MB of memory required for full-sized plots), a plotter, or a camera. In testing SlideWrite Plus I used a PC's Limited 286 PC with an EGA card, a Mitsubishi color monitor, and a Logitech mouse. The output was sent to an IBM Proprinter, HP LaserJet+ printer, and an HP 7550 plotter.

Two impressive qualities of SlideWrite Plus are the ease with which one can produce good-looking graphs and the presence of features important to scientists and engineers. Graphs are created by following a logical series of options presented in menu form. The numerical data can be entered either from the keyboard or imported from an ASCII file. (In addition, Lotus 1-2-3 graphs can be imported.) The format of the ASCII data file must be a series of columns with the x values in the first column and the y values for each curve to be plotted in the following columns. SlideWrite Plus can handle up to 4000 pieces of data per graph. For displaying multiple data sets there are six line patterns and twelve symbol types.

SlideWrite Plus has several features of particular interest to the scientist. Either or both axes can be set to log scale. Data can be plotted

against a second y axis along the right side of the graph. A second x axis can be displayed along the top of the graph but data cannot be plotted against it. Error bars can be added to four graphs using the other four data sets available for the size of the error bars. There is a provision to annotate graphs with multiple super and subscripts. SlideWrite Plus also contains a very easy to use curve fitting feature. Fits of data may be linear, exponential, log, power, or polynomial. The order of the polynomial fit can be as high as six. In addition to plotting the fit along with the data SlideWrite Plus provides a statistics page for each fit which includes statistical parameters such as the average, standard deviation, coefficients of the polynomials, and the R value of the fit.

In addition to the construction of graphs SlideWrite Plus has a draw mode in which pictures may be added to the final product. In the draw mode one can add lines, boxes, circles, arrows, text, and clip-art figures from the figure library. The introduction of these graphical annotations is controlled by the position of the cursor and a menu along the bottom of the screen. While one can do limited line, circle and box drawing, SlideWrite Plus is not for freehand drawing. Any figure that is more than a straight line, arrow, box, or circle must be imported as a clip-art figure. SlideWrite Plus comes with about 110 figures. None of the figures in the library looks to be of any use to the chemist (see comments on Figures and Fonts).

SlideWrite Plus has several convenient features for displaying or printing multiple graphs. Up to four graphs can be displayed on one page. There is also a batch print feature which allows one to print out 45 graphs with one command.

The Fonts&Figures accessory consists of ten more fonts, a library of about 300 figures, and a figure maker utility. Of the new fonts seven are improved variations of the original fonts and three (two script fonts and a gothic font) are all new. One of the nice improvements made over the original modern bold and modern light fonts is the entire Greek alphabet. Of the 300 new figures in Fonts&Figures there are eighty in the "chemistry library". Most of these figures are simple chemical structures. Fifty of the figures in the chemistry library are five- or six-membered rings with various options for heteroatoms. The most complex structure

is a steroid backbone.

Fonts&Figures also includes a figure maker so the user can add to the library. To construct a figure one must write the code for all the motions required to draw the figure. In some cases this is not too difficult but in most cases this is very time-consuming. The process is only worthwhile for figures that are either simple or that the user would employ extensively—such as a logo.

Overall SlideWrite Plus 2.1 with the Fonts&Figures accessory is very useful graphing software with many features that are often missing from packages designed with the businessman and not the scientist in mind. However, there are several limitations to SlideWrite Plus: (1) no automatic generation of x axis values given the maximum, minimum, and number of data points, (2) no ability to append ASCII datafiles to graphs already prepared, and (3) no compatible output with Matrix film cameras or CGM metafiles. If these problems are not critical to the user then SlideWrite Plus is certainly a good package at a very competitive price.

Addendum: The newest version of SlideWrite Plus (3.0) has many new features. The two most significant changes are (1) the ability to easily append ASCII data files to previously prepared graphs and (2) the capability to produce CGM metafiles and files for Matrix film devices. The many added capabilities of V3.0 (a free trial disk is available) certainly justify the \$100.00 increase in price over V2.1. SlideWrite Plus V3.0 lists at \$445.00. The upgrade costs \$95.00 to those who purchased Version 2.1 before July 1, 1988, and \$50.00 to those who purchased it after July 1, 1988.

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dms4Cite, Version 5.13. Sidereal Technologies, Inc.: 263 Center Avenue, Westwood, NJ. List Price \$295.00; \$195.00 per copy for purchases of five or more. Demonstration Only Version \$10.00.

dms4Cite (formerly Martz-BIBLIOFILE) is a software package to edit, search, incorporate into a document, and format a file of bibliographic references. The software requires a computer with PC or MS DOS, Version 2.0 or higher, an 8088, 8086, 80286, or 80386 (or compatible) CPU, and at least 128K of free memory. dms4Cite works best on a hard disk system; additional documentation (supplied by Sidereal Technologies, at extra cost) is required for operation on a dual floppy disk system. dms4Cite is available on 5 $\frac{1}{4}$ or 3 $\frac{1}{2}$ in. floppies; it is not copy protected, to allow for a personal backup copy only.

dms4Cite is designed to handle most aspects of reference citation for documents. The program allows the user to create a database of references and then select some or all of the references and incorporate them into a separate bibliographic file. dms4Cite gives each reference a unique accession number. Independently, the user can create a "parent" document with one of a variety of word processors (see below) and can cite references by using the appropriate accession number, preceded by a single left quotation mark. dms4Cite then scans the "parent" document, replaces the quotation marks and accession numbers with citations in a format suitable for publication, and creates a ".cit" file which incorporates these citations, and which can be read and printed by the word processor. Simultaneously, dms4cite uses the bibliographic file to create a "bib." document which contains all the cited references, in a style suitable for publication, and which can be read, edited, and printed by the word processor.

Each reference in the database contains fields for Author(s), Year of Publication, Title, Source (journal, book, etc.), Location (volume, pages), and Keywords. References for the database may be imported from online databases such as CAS Online, MEDLINE, and BIOSIS, or entered via the keyboard. Keyboard input of references to the database is very simple and is facilitated by a number of in-built features. Authors names can be input without punctuation or formatting in most cases, with the software performing the necessary formatting automatically. Journal names can be input as acronyms which are later replaced automatically with the correct name or abbreviation. The Keywords field may be used for the inclusion of text, so that a dms4Cite database can serve as a useful catalog of a reference collection. References for bibliographic files are

selected from the database either by accession number or by searches. All of the fields in the database may be searched, using boolean-type operations in a straightforward manner.

The way references are cited in the ".cit" file depends largely on how the accession numbers were originally typed in the "parent" document. However, dms4Cite can replace the accession number with just a reference number (as would be required for most journals in chemistry) or with an author and year (as would be required for most journals in the biological sciences).

dms4Cite can style references in the "bib." file in a wide variety of ways. The software comes with a number of style types already incorporated (most of which are for journals of the biological sciences), but user-defined styles can be added as required. For example, references can be made to include some or all of the fields listed above, in any order, and the contents of the various fields may be printed in a variety of typefaces (standard, bold, italics). References in the "bib." file may be ordered in a variety of ways, including in order of citation in the original document and in alphabetical order of authors' names.

One particularly useful feature of dms4Cite allows several "parent" documents to be scanned in turn, and the accession numbers in all of them used to compile a single "bib." file. This feature makes it possible to use dms4Cite for very large projects (theses, books) where it is inconvenient or not possible to have a single "parent" file.

dms4Cite cannot be used to incorporate references at the bottom of each page in a document. With dms4Cite, each citation in the "parent" document can only lead to a single reference in the "bib." file; it is not possible to group several references together (as, for example, ref. 1(a), 1(b), 1(c)...) and refer to them with a single citation. Also, dms4Cite cannot directly incorporate paragraphs of text into the "bib." file, as would be required in cases where notes are to be included in a "References and Notes" section of a manuscript. Paragraphs of text can, however, be inserted in the "bib." file later, using the appropriate word processor.

Most of the programs in dms4Cite can be run through a menu system (not available for the floppy disk version), a feature which inexperienced users should find particularly helpful. dms4Cite comes with a brief manual and a demonstration database, and includes a tutorial. The tutorial is straightforward, takes just a few hours to complete, and leads the user through most of the steps required to operate dms4Cite. Most of the information required to operate dms4Cite is incorporated into online Help menus, but it is not always obvious where to find the right Help menu for a given problem. A more detailed manual would be useful.

There are a few trivial bugs in the program. One particularly annoying bug is the following: when the user makes certain errors in running dms4Cite, a message is flashed on the screen, but before the message can be read, it is replaced by the main dms4Cite menu. Once recognized, these bugs are of little consequence, but they may nevertheless be troublesome to the beginner.

The manufacturer claims that dms4Cite is compatible with WordPerfect, Wordstar, and ASCII-type word processors (e.g., Final Word II, PC Write, Xywrite). Some other word processors are also supported (including DEC WPS PLUS, DisplayWrite 2, 3, and 4, Microsoft Word, Multimate Advantage II, Samna Word, Volkswriter 3, Wang PC, Wordstar 2000), but files created with these word processors must be converted to/from Wordperfect format by the Perfect Exchange package (tm Systems Compatibility Corp.; available from Sidereal Technologies for \$75.00). I tested dms4Cite with Wordstar and Wordperfect (Version 4) and found it worked well in each case. However, users may encounter difficulties associated with the idiosyncrasies of their particular word processor, and any intending purchaser should first use the Demonstration version to check that dms4Cite is truly compatible with the word processor to be used.

Overall, dms4Cite is a powerful citations management package that is easy to use. It is capable of producing bibliographies in styles suitable for publication in chemical journals. dms4Cite should prove valuable to any chemist who needs to write manuscripts with bibliographies, provided that it is compatible with the chemist's word processor.

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