

## Additions and Corrections

**Cyclobutene Photochemistry. Partial Orbital Symmetry Control in the Photochemical Ring Opening of a Constrained Cyclobutene** [*J. Am. Chem. Soc.* **1991**, *113*, 4019]. WILLIAM J. LEIGH\* and KANGCHENG ZHENG

Page 4019: The product quantum yields for direct photolysis (193 nm) of *cis*- and *trans*-**1** and for *cis,trans* isomerization of (*E,E*)- and (*E,Z*)-**2** are reported incorrectly owing to errors in the determination of GC calibration factors. The correct values (all corrected for relative GC responses) are given here in Table I. The product yields which were reported in eq 1 in the paper

**Table I.** Quantum Yields for Product Formation from Direct Photolysis of cyclobutenes *cis*- and *trans*-**1** and Dienes (*E,E*)- and (*E,Z*)-**2** in Deoxygenated Pentane Solution

substrate	( <i>E,E</i> )- <b>2</b>	( <i>E,Z</i> )- <b>2</b>	C <sub>10</sub> H <sub>16</sub> isomer	<i>cis</i> - <b>1</b>	<i>trans</i> - <b>1</b>
<i>cis</i> - <b>1</b> <sup>a</sup>	0.48 ± 0.06	0.14 ± 0.02			
<i>trans</i> - <b>1</b> <sup>a</sup>	0.08 ± 0.02	0.45 ± 0.06	0.04 ± 0.01		
( <i>E,E</i> )- <b>2</b> <sup>b</sup>		0.20 ± 0.03		0.05 ± 0.01	
( <i>E,Z</i> )- <b>2</b> <sup>b</sup>	0.27 ± 0.03		0.009 ± 0.002		0.019 ± 0.004

<sup>a</sup> From photolysis of 0.02 M solutions with 193-nm light, using the ring opening of bicyclo[4.2.0]oct-7-ene to *cis,cis*-1,3-cyclooctadiene ( $\Phi = 0.12 \pm 0.02$ ) as actinometer.<sup>1</sup> <sup>b</sup> From photolysis of 0.02 M solutions with 254-nm light, using the *cis,trans* photoisomerization of *cis,cis*-1,3-cyclooctadiene as actinometer.

were calculated from relative GC peak areas and were not corrected.

The distribution of (*E,E*)- and (*E,Z*)-**2** obtained from direct photolysis of *cis*-**1** ((*E,E*)-**2**/*(E,Z)*-**2** = 3.4 ± 0.6) compares favorably with the distribution expected from disrotatory, adiabatic ring opening ((*E,E*)-**2**/*(E,Z)*-**2** = 3.7 ± 0.8). In the case of *trans*-**1**, the observed and predicted distributions are (*E,Z*)-**2**/*(E,E)*-**2** = 5.6 ± 1.1 and *E,Z*-**2**/*E,E*-**2** = 2.6 ± 0.4, respectively. The main conclusions of the paper are unaffected by these errors.

(1) Clark, K. B.; Leigh, W. J. *J. Am. Chem. Soc.* **1987**, *109*, 6086.

## Computer Software Reviews

**Library Master. Version 1.24.** By Harry Hahne. Balboa Software: 61 Lorraine Dr., Willowdale, Ontario M2N 2E3, Canada. (416) 730-8980; fax (416) 730-9715; e-mail address hahne@epas.utoronto.ca). List price: \$199.95, \$599.00 for a 5 node, local area network version (demo version available for \$5.00).

Library Master is a powerful and well-designed program for managing bibliographic and textual information. It aims to simplify bibliography creation and management by incorporating characteristics of word processing and text database programs. Library Master succeeds in providing extensive functionality while keeping the operation simple, straightforward, and consistent throughout. The flexibility of the program makes it well suited for a broad range of applications, including notetaking and report writing, organizing references and maintaining bibliographies, and building personal databases from information obtained from online searches or CD-ROM citations. Each step of the text management process is handled effectively. Data is input with a capable editor or by using the separate text importing program. Powerful routines exist for manipulating textual information such as searching for relevant citations, sorting for subsequent output, and browsing for idea generation. Bibliographies or reports may be generated easily with many options, including producing output in common word processor formats.

Installation and setup of Library Master are easily accomplished. The program requires an IBM PC or compatible with DOS 2.0 or higher and 384K (512K is recommended). The installation program guides the user through the process in standard English phrases. After transferring all appropriate files, the setup program is called up to set initial program defaults. The LIBSETUP program is also available to change printer and word processor parameters and program defaults, such as screen colors, file paths, and Library Master editor parameters. The software comes with extensive online help documentation and a comprehensive User's Manual. All aspects of the program are well explained, although the value of the User's Manual as a reference guide is limited by inadequate indexing. Balboa Software provides excellent technical support, available by telephone or Internet e-mail.

Several general features of Library Master make it a pleasure to use. Each screen has a useful status line at the top and indication of all available function keys along the bottom. The status line shows information about the process the database is currently executing and whether the editor is in insert or overwrite mode. One moves about the program following consistent, clear menus. Function selection can be made three

ways: typing the number of the selection, typing the first letter of the selection description, or using the cursor to bring the highlighted box to the desired selection. (A Microsoft mouse can be loaded with the standard mouse menu and used to select items on some menus, but further customization is desirable using the MENUMAKE kit available from Microsoft. Other commercial mice can probably be used also. An MS Windows version of Library Master is being considered by Balboa Software.) Other point-and-select menus are abundant, including those for database, search field, or output format selection. The up-cursor or F2 key consistently brings one up to the selection screen. Library Master also has available some useful customization features, including definition of colors of screen areas and keystroke macros for combining multiple keystrokes into single keystroke functions.

With Library Master you can begin immediately to develop databases. It comes with seven databases to use as models for a variety of applications. Databases can be of practically unlimited size, with a capacity of up to 65000 records. Each of these can be up to 65000 bytes long. The prototypical bibliographic database, BIBLIO1, has 24 predefined record types, but up to 50 can be defined in each database. One omission for scientists is a patent record type. For journal articles, there are 39 predefined fields, and a total of 50 may be defined for the database as a whole. The variety of field characteristics is a major strength of Library Master. Fields may be of variable and nearly "unlimited" size. They may be defined as dates (numerous formats and ranges acceptable), names, integers, text, text with paragraphs, and literature references (i.e., citations to which the database record refers). Fields can be further characterized as lists, unique values, required values, containing subfields, or indexed for improved searching. Data input is facilitated by the Data Input Form which provides at a glance (possibly over several screens) the structure of a record, with an information field name beside or above the input area. This form is readily modified so that database structure can evolve.

The editor is used to input new data and modify old records. Getting around the Data Input Form is straightforward and is further aided by a jump-to-selected-field option. Editor commands are generally mnemonic combinations of the ALT or CONTROL keys with alphabetic keys in the style of the WordStar word processor. For example, use <ALT C> for copy a block to the paste buffer or <ALT B> for turn on bold-faced. Editor commands include font changes (underscoring, italics, bold-faced, sub- and superscripts), search and replace, block commands,

paste buffer, and various miscellaneous functions. Case control is due in a future version.

Data may be imported from almost any source with defined record format using the LIBIMP program. Field delineated output from STN or other database vendors is ideal. At least nineteen sample import parameter files are provided, including generic Dialog Information Services files, Current Contents online and on diskette, and Pro-Cite output. An import format parameter file for the Chemical Abstracts File on STN was straightforward to create, but Library Master anticipates making one available soon. Library Master handles importing multiple record types by requiring the document type field to lead the record; therefore, the downloaded output must be edited to relocate the "DT" field to the top of each record. Additional shortcomings, which are being addressed by Balboa Software, involve field parsing. For example, author and literature source fields often contain multiple entries. At present, Library Master considers names as consisting of only two parts, last names and all else; "first" names may include middle names or initials. For literature source, Library Master cannot, at this point, separate journal name, volume, issue, pages, dates, etc. from a single source ("SO") field. However, after editing these fields in the Data Input Form, the program will produce appropriately formatted bibliographies and reference lists.

Database content may be searched globally or for contents of specific fields. The Search input screen includes a list of the database's field types for selection and use as search criteria. Selection of an indexed field automatically shows a list of all indexed entries. Field contents can be truncated in the search, and multiple criteria combined with Boolean "and", "or", or "not" operators; numerical "less than", "greater than", "equals", or combination operators; or "approximate" when spelling is unclear. Searching is fast, as Library Master uses "B-tree" indices. However, these may be awkward to most searchers of Chemical Abstracts in which individual words and registry numbers are searchable. In the B-tree, all index entries are phrases, so terms not found at the beginning of the field must be surrounded by preceding and following truncation symbols. Library Master allows separate index fields in the CA file to be read in as separate entries in a "list" index term field, but there is no proximity operator to allow linking of registry numbers with related text descriptors. The records selected as the result of a search may be stored as a record list for later handling.

An entire database or various types of subsets can be effectively and efficiently browsed, deleted, sorted, merged, and repaired. Both browse and delete modes can work on the whole database, a record list from a search, records selected by the contents of indexed fields, or individual

records. The browse function gives access to the entire record via the Data Import Form. However, the record is protected from change during browsing. Should editing be desired, a useful keystroke macro is provided in the User's Manual which switches from browse to edit modes on the same record. Another macro can be written to return to browse mode. Sorting, part of the report generation mode, uses a Sort Order File to designate which of up to three fields will be used in the sort and whether the sorting is ascending or descending on each field. Sort parameters must be set up for each applicable record type. Entire databases or record lists are readily merged into the current database. If the source and destination databases do not have identical structure, Library Master will make some adjustments to make the incoming data fit into the destination database. The manual warns that under these circumstances, "some bizarre results may occur". In any event, repair functions exist to undo the damage, either from this situation or other occurrences such as disk error, loss of power, or rebooting while a database is open.

Report generation is a full-featured function designed to produce a variety of reports from the seven supplied databases. Reports may be sent to the monitor, the printer, or to a disk file. Parameters for twelve printers and eight text editors or word processors are currently supplied, and most of these parameters can be modified using the LIBSETUP program. Among the word processors available are WordPerfect, Microsoft Word, and WordStar. Formatting reports is a two-step process. Individual bibliographic citations use Style sheets, of which 10 are supplied, including standards Turabian and Chicago. Modification of Style sheets is straightforward, so other styles (such as the one for this journal) can be readily created. A clever feature is the ability to preview references in the selected style during the record editing process. The overall report structure is defined by the Format file. The nineteen Format files supplied include those for a full formatted bibliography, annotated bibliography, and mailing lists, labels, and envelopes. While Library Master can output reports in formats which can be directly imported into word processors, it cannot interact with word processor programs to create footnotes "dynamically" during the article writing process, as some specific reference handling programs can.

In summary, Library Master is a well-designed textual database management program. It is economical, easy, and pleasant to use and versatile for many applications. While the number of such programs has grown, Balboa Software has clearly been evaluating other programs while developing one that they personally like to use. It is time for some of the other program developers to look at Library Master to see how so much can be done well.

Thomas E. Wolff, Amoco Corporation

## Book Reviews\*

**Structure and Bonding 75. Long-Range Electron Transfer in Biology.** Edited by G. A. Palmer (Rice University). Springer-Verlag: Berlin. 1991. 233 pp. \$98.00. ISBN 0-387-53260-9.

Few chemists escape graduate school without exposure to the mysteries of the "inverted region" or the yang and yin of through-bond vs through-space coupling. *Structure and Bonding 75* applies these and other constructs of electron transfer theory to biological electron transfer reactions, providing a useful snapshot of the chemists' approach to this field.

The profusion of review articles and books on electron transfer reactions reflects the central role that these reactions play in chemistry. Three useful volumes have appeared in 1991 alone: the above, *Metal Ions in Biological Systems 27: Electron Transfer Reactions in Metalloproteins* (Dekker Press), and *Electron Transfer in Inorganic, Organic and Biological Systems* (ACS Advances in Chemistry Series No. 228). There is considerable overlap in the scientific content of the books, which are mostly updates of individual experimental research programs that utilize modified and native proteins as well as model electron transfer compounds to probe the relationship between structure and function in these reactions.

*Structure and Bonding 75* is distinct from the other books in its inclusion of two fairly general theoretical reviews by P. Bertrand and by A. Kuki. Five reviews of experimental approaches from the groups of B. M. Hoffman, H. B. Gray, A. G. Mauk, G. McLendon, and A. G. Sykes follow. These papers describe biological electron transfer experiments

on protein complexes, ruthenated metalloproteins, genetically engineered electron transfer proteins, bimolecular electron transfer systems, and blue copper proteins, respectively. Consisting mostly of already published data, the experimental reviews do provide excellent perspectives of multiyear research programs, often absent from the stream of communications on these subjects. The papers in this volume, and the abundant references throughout, should help the uninitiated identify important current research challenges.

The focus of *Structure and Bonding 75* is on chemically modified or genetically engineered proteins. Its limited length prevents it from providing a comprehensive survey of the electron transfer field. For example, little discussion of work on the photosynthetic reaction center or solvent friction is present. This book should be a helpful resource for students initiating research on electron transfer reactions. The articles are typeset, nicely illustrated, and, in general, clearly written and sharply focused on one or two aspects of the problem. A sense of the wide variety of productive theoretical and experimental approaches to this subject is conveyed by these seven papers.

David N. Beratan, California Institute of Technology

**Modern Pulsed and Continuous-Wave Electron Spin Resonance.** Edited by Larry Kevan (University of Houston) and Michael K. Bowman (Argonne National Laboratory). John Wiley & Sons: New York. 1990. ix + 440 pp. \$95.00. ISBN 0-471-50274-X.

Pulsed, high frequency, and imaging electron paramagnetic resonance techniques have undergone dramatic and important changes in the past five years which merit review such as provided by the anthology edited by Kevan and Bowman. This collection consists largely of reviews of

\*Unsigned book reviews are by the Book Review Editor.