

Additions and Corrections

Hydrosilylation–Allylation Sequence for the Stereoselective Elaboration of β -Hydroxy Esters [*J. Am. Chem. Soc.* **1992**, *114*, 2745–2746]. ANTHONY P. DAVIS* and STEPHEN C. HEGARTY

Table II: The header for the final column, ratio 6:7^c, should read ratio 3:4^c.

Electron Transfer in Bis-Porphyrin Donor–Acceptor Compounds with Polyphenylene Spacers Shows a Weak Distance Dependence [*J. Am. Chem. Soc.* **1992**, *114*, 6227–6238]. ANNA HELMS, DAVID HEILER, and GEORGE MCLENDON*

Detailed synthesis descriptions on pages 6229–6238 intended for deposition into Supplementary Material inadvertently appeared in the Experimental Section of this paper as textual material.

Several of the compound preparations listed in the supplementary synthetic material were inadvertently improperly referenced. In particular, syntheses of **15**, **35**, **36**, and **37** were first reported by Staab and Haenel (*Chem. Ber.* **1973**, *106*, 2190–2202). We regret the error in excluding reference to this work.

Computer Software Reviews

OneScanner. Apple Computer, Inc.: 20525 Mariani Ave., Cupertino, CA 95014-6299 (800-538 9696), bundled with **Ofoto Version 1.0**. Light Source, Inc.: 500 Drakes Landing Road, Greenbrae, CA 94904-9936. List price \$1379.00 (educational or government price \$965.00). Includes terminator cable and hyperscan software. OneScanner requires System 6.0.7 or later and includes 32-bit QuickDraw; Ofoto requires 1 MB RAM with System 6.0.7 (2 MB with System 7) and LaserWriter driver Version 6.0.5. **OmniPage Professional 2.0.** 100 Cooper Court, Los Gatos, CA 95030 (800-535 7266); requires scanner, Mac with 68020 or 030 chip, **4 MB RAM; hard disk.** List price \$995.00 (MacWarehouse \$649.00).

Anyone preparing electronic manuscripts on a regular basis will frequently need to incorporate large amounts of material that is available (to them) only in printed format. An extensive list of literature references to topics of interest is discovered, perhaps for inclusion in a personal database; experimental results from a research group member's thesis need updating; "pre-PC" teaching notes and other class materials need "punching up" with illustrations; photocopies of major last-minute changes to an article are received from a co-author. All could require tedious retyping of page after page of text, but why not convert directly from the printed page into your PC?

The Apple OneScanner is a recent entry into the desktop publishing environment. Anyone who has used a photocopier will understand the logistics of operating the OneScanner. This flatbed scanner accepts legal-sized originals, will scan and print at resolutions up to 300 dpi, and can process simple text as well as more complex graphics and photographic images at 8 bits (256 greys). Launching Ofoto produces a pop-up window that allows users to either customize scan parameters (brightness, contrast, image type, resolution) or accept defaults and let the software decide what is being scanned. A handy Prescan option quickly determines the original's size and allows the user to select a specific portion for full scanning (e.g., text excluding chemical structures). We found this option more useful and faster than the Autoscan mode, which includes automatic straightening and cropping routines. After an image is scanned, it can be cleaned up, if necessary, and edited at the pixel (Fat Bits) level, sharpened, inverted, rotated, or resized and saved in a variety of formats (PICT, TIFF, EPS, MacPaint) recognizable by your favorite image processing software. Output may be configured for a number of different devices (printers, fax modems, etc.). To process text images, they must be converted by an Optical Character Recognition (OCR) package into a file that a word processor can manipulate.

Our setup consisted of a Macintosh IIfx with 16 MB of RAM connected to a LaserWriter IINT and 80 MB internal and 175 MB external hard drives running System 7.0, Ofoto, Microsoft Word 4.0/5.0, and OmniPage Professional 2.0, one of several top-rated OCR packages. Under these conditions, all file transfers and conversions took place with no memory problems. Laser-printed, typeset, first-generation photocopy, typewritten, and dot-matrix originals were scanned; faxed documents, not surprisingly, produced mixed results. Typically, a full page of text or 8 × 10 in. photo required about 10 s for a prescan and 1 min for a full scan. OmniPage Pro recognizes TIFF-format files, which naturally become larger as the size and complexity of the scanned image increases. Typical scans of single-page text gave TIFF files of about 1 MB; for large photos or other more complex images that require more greys, file sizes can reach 8 MB. These bulky files are transformed into much smaller (e.g., 10 KB) text files in just a minute or two (more time was needed for recognition of small-type, multiple-column originals).

The success of transforming the printed word into electronic form depends not only on the quality of the original and of the scanner but also on the abilities of the OCR package. A useful text conversion program should handle a wide variety of printed originals and include options for saving output in formats "readable" by the large number of word and image processors on the market. It should also be "trainable"—that is, it should allow recognition of unusual characters or alphabets (Greek characters in the Symbol font) to avoid repetitious proofreading corrections. With OneScanner and Ofoto, clean and moderately dark originals—even photocopies and dot-matrix documents—gave consistent high-percentage conversion results using OmniPage Pro. Print manuscripts produced using a minimum number of fonts and larger type will convert more quickly—and sometimes more cleanly—than those with several typefaces in smaller font sizes. The infrequent "l vs 1 vs I" or "S vs 5" error occurred in alphanumeric text; incomplete or weakly formed characters were sometimes unrecognized; documents with markedly varying paragraph margins and formats sometimes produced mixed results when converted in "Automatic" mode, but this can be helped using the customizing features in the OCR package. The most consistent quirk found involved literature references produced with mixed bold, italic, and plain text; although the text itself survived the conversion, some bold/italic attributes needed reformatting. However, anyone who has typed in references, and realizes what a tedious and error-prone task this can be, will likely accept this minor "problem". The OneScanner's lid has

enough "play" to accommodate half-inch thick originals, and can be removed for larger bound books. Success in scanning large library-type bound volumes varies as with photocopiers (anyone who has tried copying from thick journal volumes with impossibly narrow margins will get the idea).

These powerful tools are not without some disadvantages. The OneScanner does not have an automatic feeder, which can make swapping of originals somewhat tiresome. As described above, the process currently involves three distinct steps; Caere has recently announced the upcoming release of OmniPage Direct for the Macintosh, which will convert images and automatically save text in a pre-selected word processing format in a single step. Significant memory is needed to operate this software, even at the most basic level—Ofoto (2.5 MB) and OmniPage Pro (4.5 MB) together require 7 MB of RAM, and more RAM is needed to run the word processing software at the same time (although that is not necessary; all scanning can be done first, and final conversion performed later). Also, hard disk memory is quickly gobbled up by even simple images, requiring frequent file weeding if storage space is at a premium. In short, if you have a very basic Mac setup, an upgrade will be necessary, and the OCR software (typically \$600–\$1000) is an added expense.

For those who can afford the investment, however, the ease with which pre-prepared charts, schemes, photographs, and clip art (otherwise unobtainable in electronic format) can be used to improve the look of even the simplest of documents makes the OneScanner quite attractive. Its advantages will be all the more obvious to the "two-fingered typist" who must repeatedly "pull together" and revise text from printed sources. It is, simply, a tool which will increase in value as the chemist becomes the desktop publisher.

Mark Volmer and Albert Padwa, *Emory University*

HMO. Version 2.0. Trinity Software: P.O. Box 960, Campton, NH. List price \$95.00; site license for up to 10 copies on a network server \$295.00; site license for up to 30 copies on a network server \$495.00.

HMO is a Huckel molecular orbital program with a graphical front end. It is compatible with both MS-DOS machines and Apple Macintoshes. Under both operating systems, the memory and disk space requirements for running HMO are minimal.

The software was tested on the Macintosh SE with 1 MB of memory, as well as on a Macintosh IIcx with 8 MB of memory. A non-post-script laser printer was used as the output device. System installation was straightforward and clearly explained in the accompanying manual. Only 200K of disk space were required, and the program could be run equally well from the floppy drive and the hard drive. Molecule building was easily accomplished by following the examples given in the manual or by editing one of the large number of sample structures included with the program. Several options for displaying the results are provided, and these, along with the graphical interface, are the major strength of the program. The molecular structure is displayed and indexed for every output type. All references to properties are related to the indices,

making interpretation of the results simple and unambiguous. A reasonably broad range of heteroatoms (B, N, O, S, F, Cl, Br) is supported. Two sets of atom parameters are included in the code (Streitwieser's set¹ and zeroth order parameters). Atom and bond parameters can both be modified by the user. Again, the documentation of this point is clear and easy to follow.

The principal disadvantage of the current implementation of HMO is that there are not cut and paste features. It would be useful to be able to copy diagrams and tables out of the output and paste them into other documents. Another feature that would extend the utility of HMO on either the Macintosh or the MS-DOS platform would be the addition of the extended Huckel (EHT) algorithm to the program. The current version supports only π -electron calculations. Programs which incorporate EHT algorithms are available for the Macintosh and the IBM from the Quantum Chemistry Program Exchange² at a price comparable to the HMO system, but typically do not have the nice graphical front end.

The MS-DOS version was tested on a Toshiba laptop with 512K of memory, an optical mouse, and graphics capability. A Microsoft compatible mouse and a graphics card and monitor are required to run HMO. The program had much the same feel under MS-DOS as it had on the Macintoshes. The documentation is concise, but clear.

This program would be most useful for research groups that are looking for something slightly more sophisticated than the "back of the envelope" that they might have been using for Huckel calculations on organic systems. It could also find a place in the undergraduate teaching curriculum, in organic chemistry or physical chemistry courses that cover Huckel theory. In summary, HMO is easy to learn and inexpensive and can be run on platforms available on most campuses and in most research groups.

(1) Streitwieser, A. *Molecular Orbital Theory for Organic Chemists*; Wiley: New York, 1961.

(2) QCPE, Creative Arts 181, Indiana University, Bloomington, IN 47405.
Michelle M. Francl, *Bryn Mawr College*

HMO. Version 1.3. Dr. Allan Wissner, Department of Oncology and Immunology, Medical Research Division, American Cyanamid Company, Lederle Laboratories, Pearl River, New York 10965. Free.

HMO is a free program, available from the developer (send an 800K, formatted disk and a self-addressed, stamped return envelope to Dr. Wissner). The program runs on a variety of Macintosh computers and is compatible with multifinder running under systems 6 and 7. It has a convenient graphics interface and is otherwise quite user-friendly. The output includes the following: eigenvectors; charge densities; electron density–bond order matrix; electrophilic, radical, and nucleophilic superdelocalizabilities; and energy level and eigenvector diagrams. While it is the policy of this Editor not to review free software (or shareware), this package is unusually well done and can be recommended.

Book Reviews*

The Chemical Synthesis of Peptides. By John Jones (Oxford University). Clarendon Press/Oxford University Press: Oxford and New York. xi + 228 pp. \$75.00. ISBN 0-19-855643-8.

Dr. Jones prepared the text not only in a chronological and scientific style but also with an overview and appreciation of the field with a choice of language and literary skill which makes the text both intellectual and very pleasant to read.

For example, he writes of the proteins that they are "natural polymers which are assembled under nucleic acid control from a menu comprising 19 L- α -amino acids". He also conceives of these proteins as "the very stuff of life, they are present in abundance and diversity in every part of every living thing on Earth".

He estimated that, at present, there are at least 5000 chemists engaged full time in research on peptides and proteins. For these multitudinous chemists, this book is timely.

For peptide synthesis, α -amino protection and α -carboxy protection are surveyed and followed by the organic chemistry of diversified peptide bond formations.

Residue-specific considerations then follow, and the unusual amino acids are not neglected, including N-methyl- α -amino acid, and others.

Perhaps the main theme of the book is on the synthesis of ordinary peptides and proteins in terms of strategy and tactics and then on solution

peptide synthesis, solid phase peptide synthesis, and the Sheppard approach.

The book concludes with the synthesis of conjugated peptides, simple cyclo peptides, and more complex modified peptides.

Adding to the fascination of reading his account of the chemical synthesis of peptides is his tribute to the many pioneers in this field by citing their stepwise discoveries, beginning with Emil Fischer in 1906 and then appropriately the many chemists who followed including Bergmann and Zervas, Rudinger, Sheehan, Brenner, DuVigneaud, Merrifield, Hirschmann, and many others.

His Epilogue is a reflection on the future which gives credit to Rudinger and Hirschmann on predicting the stimulation of discoveries on peptide-releasing factors, new instrumentation including HPLC, high-field FT-NMR, recognized by Veber, and FAB-MS. He justifiably credits advances due to technology as well as to novel chemistry.

He visualizes the future including chemical synthesis of artificial enzymes, asymmetric synthesis, glycopeptide synthesis, and even synthetic vaccines.

This book by Dr. John Jones is highly commendable.

Karl Folkers, *The University of Texas at Austin*

Biomaterials. Novel Materials from Biological Sources. Edited by David Byrom (Biological Products Division, ICI). Stockton Press: New York; Macmillan Ltd.: Hampshire, UK. 1992. viii and 365 pp. \$100.00. ISBN 1-56159-037-1.

*Unsigned book reviews are by the Book Review Editor.