Additions and Corrections

Ab Initio Calculations Predict a Singlet Ground State for Tetramethyleneethane [*J. Am. Chem. Soc.* **1987**, *109*, 930]. PING DU and WESTON THATCHER BORDEN*

Mislabeling of an output file resulted in our erroneously reporting that the triplet UHF geometry of lowest energy for the title compound has a dihedral angle of $\phi = 44.9°$ between the planes of the allyl groups. The triplet UHF minimum actually occurs at a D_{2d} geometry, where the dihedral angle is twice this size. However, the calculations at the geometry labeled "triplet minimum" in Table I were, in fact, performed at $\phi = 44.9°$, and, as we reported, at both the ROHF and SD-CI levels the triplet minimum occurs near $\phi = 53°$. We thank Professor Ken Jordan for pointing out to us that we had misreported the location of the UHF triplet minimum.

Computer Software Reviews

Scientific Reference System II. Version 1.0. Trinity Software: P.O. Box 960, Campton, NH. List Price $125.00; Research pack (10 copies with manuals) $625.00; Network version (1 disk and manual, 10 users) $325.00. Not copy protected.

Scientific Reference System II (SRS II) is a personal database system for searching scientific references obtained as text files from online searches of databases such as CAS-Online. It is a HyperCard 2.0 stack and will run on any Apple Macintosh computer with a minimum of 1 mB RAM, System 6.05 or later, and HyperCard 2.0 or later. A hard disk is recommended for optimal performance. SRS II uses the Geneva font extensively, or Helvetica if font substitution is allowed, and Geneva is not available. The home stack supplied with the software requires Hyper-Card 2.0. The original SRS II disk as supplied is fully supported by Trinity Software. SRS II is a redesigned version of the original software with improved search capabilities, greater flexibility, and reduced stack sizes. A 46-page user manual is provided, which contains a tutorial, description of the stacks, and instructions for installation and use. No IBM PC-compatible version is available at this time.

This software is designed to organize personal files of literature references and eliminate much of the mechanical drudgery associated with hand sorting journal citation materials. It can import text (ASCII) files received from STN CAS-Online, BIOSIS, and CAB; Dialog CAS-Online, MedLine, BIOSIS, PaperChem, and CAB; BRS CAS-Online and MedLine; Current Content on diskette, Science Citation Index (SCI) and MELVYL (the University of California system), and the Silver Platter MedLine and Agricola databases (CD ROM). SRS II is generally optimized for use with the STN CAS-Online service, but it will read text files generated by the other databases mentioned above with minor modifications. Once references have been added to the database one can edit, annotate, index, sort, and search them using the buttons and pop up menus provided. Molecular structures or other artwork can be added to a reference using the Macintosh Clipboard desk accessory. A typical use might be to flag all the references (cards) in the database (stack) which are cited in a manuscript being prepared and save them as a text file. SRS II will create the file in the format required by the selected journal. A large number of journal formats in chemistry, biology, and medicine are provided. Fairly sophisticated Boolean searches can be performed based on key words provided by the database, and/or strings and index terms created by the user. Up to ten index terms can be created for each citation and comments can be added to each card in the stack.

The software works best if there is 2 mB or more of memory available.

Insufficient memory problems occurred when the package was installed on a Mac Plus with 1 mB of memory, and INIT files had to be removed from the System file. When the tutorial program was run, several attempts were necessary to load the required files. However, installation on a Mac II with 5 mB went smoothly and rapidly, and no operating problems were subsequently seen. If the user is familiar with the HyperCard application package, the program can quickly be mastered after an hour or less with the enclosed tutorial. For those unfamiliar with the logic and operation of HyperCard some frustration is likely to occur, since the tutorial text instructions are unclear at several points: "click on a button" in several cases means to click and drag to open a pop up menu, rather than simply point and depress the mouse button; the different results produced by using the return key and the arrow keys are not fully explained. Some command sequences do not produce the desired results when manipulating the stacks. If the user is not familiar with the Macintosh hierarchical file system, other problems can occur when attempting to open or save files or stacks. Those unfamiliar with Hyper-Card should use the tutorial/demo supplied with that application before using SRS II.

Loading an ASCII text file containing 171 citations created by STN CAS-Online into a HyperCard stack in SRS II took about 25 min. The text file was a real-time file containing log-in information, commands, and other information on search parameters. SRS II ignored command/response strings and correctly recognized citation, author, abstract, etc. information for all citations and placed it in the appropriate card fields. This recognition capability eliminates the need to edit real-time files to remove unwanted strings. No structural information is included in text files, but it was easily added with the Macintosh Clipboard desk accessory. Structure searches cannot be done. We were able to rapidly search for citations containing selected words, character strings, article key words, and our own added index terms. We easily created substacks of citations, added new cards to the stack by hand, and printed reports. These software tasks were executed rapidly and smoothly on the Mac II, but they were noticeably slower on the Mac Plus.

SRS II is not specifically oriented to academe or industry but rather toward online database users who must organize and search journal citation information. It efficiently produces complex searches and reports based on author, publication data, patent, key word, etc. SRS II can be customized to suit individual searching and reporting needs. The citation formatting feature is very useful for conveniently adding references to a manuscript.

William V. Willis, *California State University, Fullerton*