Computer Software Reviews

component with respect to the other in a [2]rotaxane, the technology for building "molecular machines" will emerge.

The molecular shuttle described in this communication is the prototype for the construction of more intricate molecular assemblies^{2,16} where the components will be designed to receive, store, transfer, and transmit information in a highly controllable manner, following their spontaneous self-assembly^{17,18} at the supramolecular¹⁹ level. Increasingly, we can look forward to a "bottom-up"

(16) For a recent communication on the ordered threading of molecular components, see: Anelli, P. L.; Ashton, P. R.; Spencer, N.; Slawin, A. M. Z.; Stoddart, J. F.; Williams, D. J. Angew. Chem., Int. Ed. Engl., in press.

(17) For an outstandingly good review of self-assembly in synthetic routes to molecular devices, see: Lindsey, J. S. New J. Chem. 1991, 15, 153-180.

approach to nanotechnology²⁰ which is targeted toward the development of molecular-scale information processing systems.

Acknowledgment. This research was supported by the Agriculture and Food, and Science and Engineering, Research Councils in the United Kingdom and by Consiglio Nazionale delle Ricerche in Italy.

(18) For a review of self-assembly in organic synthesis, see: Philp, D.;

(10) 1 of 1. F. Synlett, in press.
(19) (a) Lehn, J.-M. Angew. Chem., Int. Ed. Engl. 1988, 27, 89–112. (b) Lehn, J.-M. Angew. Chem., Int. Ed. Engl. 1990, 29, 1304–1319.
(20) Artificial Life; Langton, C. G., Eds.; Addison-Wesley: Redwood City,

CA, 1989.

Additions and Corrections

Asymmetric Synthesis Using Diisopropyl Tartrate Modified (E)and (Z)-Crotylboronates: Preparation of the Chiral Crotylboronates and Reactions with Achiral Aldehydes [J. Am. Chem. Soc. 1990, 112, 6339-6348]. WILLIAM R. ROUSH,* KAORI ANDO, DANIEL B. POWERS, ALAN D. PALKOWITZ, and RONALD L. HALTERMAN

Pages 6344 and 6345: The ¹H NMR data reported for (R,-R)-diisopropyl tartrate (E)-crotylboronate (2) and (R,R)-diisopropyl tartrate (Z)-crotylboronate (3) were measured in C_6D_6 , and not in CDCl₃ as indicated in the tabulated spectroscopic data. ¹H NMR data for these reagents measured in CDCl₃ are as follows: 2 (500 MHz, CDCl₃) δ 5.42-5.53 (m, 2 H), 5.11 (septet, J = 6.5 Hz, 2 H, 4.77 (s, 2 H), 1.83 (br d, J = 5 Hz, 2 H), 1.64 (br d, J = 5 Hz, 3 H), 1.28 (d, J = 6.3 Hz, 12 H); 3 (500 MHz,CDCl₃) δ 5.47-5.58 (m, 2 H), 5.11 (quintet, J = 6.5 Hz, 2 H), 4.76 (s, 2 H), 1.83-1.92 (m, 2 H), 1.61 (d, J = 5 Hz, 3 H), 1.28(d, J = 6.3 Hz, 12 H).

Computer Software Reviews

The MSDS Solution (TMS) and SCS Access, Version 1.05. Logical Technology, Inc.: 5113 North Executive Drive, Peoria, Illinois 61614. List Prices: MSDS Solution \$995.00; SCS Access \$470.00; both \$1365.00. The MSDS yearly maintenance is \$205.00, while the SCS Access yearly subscription is \$495.00. A network version is also available for an additional \$850.00.

These software packages require minimally an XT (LTI recommends an AT) class IBM PC (or 100% compatible) with 640K RAM and a 20M hard disc operating with DOS 2.0 or higher. The MSDS Solution is a menu-driven outline program that allows one to enter information from a manufacturer's material safety data sheet (MSDS) into an organized format for easy filing and rapid information retrieval. OSHA's Hazard Communication Standard established the sensible guideline that all workers must have access to the safety information encapsulated in the MSDSs. Since the "worker's right-to-know" is geared more toward the industrial workplace, this software package is likely to have more application in industrial and government labs than in academia. (However, with OSHA's "Occupational Exposure to Hazardous Chemicals in Laboratories" there is currently a need in every laboratory.) The MSDS Solution allows these data to be quickly retrieved by a variety of means, including formula, product name, manufacturer, or MSDS number. Each MSDS is given a status assignment as either pending, current or non-current, or per the chemical's status in the inventory. There is a user hierarchy, allowing progressively more access and editorial power to higher ranking users. A "General User" may read current and noncurrent MSDS's and may utilize SCS Access to compile reports from the database. "MSDS Entry Personnel" may load and edit MSDS's and the

"Coordinator" may alter the status of MSDS's, assemble user lists, and import/export MSDS's.

The format of the MSDS has fields for specific information, including manufacturer's product information, physical and chemical properties, fire and explosion data, and component information, and space is set aside for comments.

Installation of the software is simple. The demo version of the program took 7 min to load on an IBM PS 2. The complete version took a little longer. (LTI reports that in the newest version they have the loading time to 2-5 min, depending on hardware.) Initially, we had some minor difficulties in getting the loaded software to run. A phone call to Logical Technology, Inc. resulted in helpful coaching.

The failure of the loaded software to run was a result of insufficient working memory due to memory resident programs. This intolerance of other resident programs is a potential downfall of this software (albeit a very small one). Given the size of many companies' chemical inventories and the number of MSDS's that would be stored in this type of data base, dedication of a PC may be recommended anyway and at any rate is a small price to pay for this organization, speed, and convenience. The smaller companies, or those with relatively small chemical inventories, who may wish to use their PC's in multiple capacities, will need to turn off any memory resident programs to run this system.

A time-saving option would be the ability to down load commercial (e.g. Aldrich) MSDS files into this data base. However, apparently electronic MSDS's have not been standardized industry wide and it was the opinion of the helpful soul at Logical Technology, Inc. that such importing would not be possible without additional programming. So, for the time being, it is necessary to enter the MSDS data by hand. For similar MSDS's, it is possible to copy and edit an existing MSDS in order to avoid having to type duplicate information. LTI also offers the electronic loading of the 2600 + Cameo MSDS's written by the Chemical Manufacturer's Association and offered through the National Oceanic & Atmospheric Administration.

The SCS Access provides federal and state listings of regulations and hazards for over 10 000 chemicals. SCS Access is updated quarterly, making it possible to stay current in the myriad of regulations that exist for chemists today. This valuable database provides chemical information, sources, changes since the last update, and comparisons to the MSDS listing. It is possible to search these entries by chemical name, CAS Registry Number, source, sequence number, or premanufacture notice number.

The supporting documentation for TMS/SCS Access is well organized and rife with examples. Detailed, step-by-step instructions are provided for searching, making queries, writing reports, and importing and exporting MSDS's with other TMS facilities. Usually, the lack of an index in the supporting documentation leads to a great deal of frustration when it comes time to actually use a software package; however, the organization and clarity of the TMS user's manual obviated this trauma (a most welcome deviation from the norm).

In a simpler (and more naive) day and age one could just bottle the wastes of research and bury it. Today, a higher conscientiousness and a vastly more convoluted regulatory framework require that we chemists deal with our wastes in a more responsible fashion. With all of the different agencies that we must now answer to, the regulatory side of things can be complicated indeed. The MSDS Solution provides for rapid organization and retrieval of safety data and the SCS Access offers a timely and convenient summation of the information and regulations necessary to handle, store, and dispose of our chemicals safely and responsibly. This software fills a valuable niche.

Glen E. Fryxell and M. A. Lilga, Battelle Memorial Institute

Book Reviews*

Biological Trace Element Research: Multidisciplinary Perspectives. ACS Symposium Series 445. Edited by K. S. Subramanian (Health and Welfare, Canada), G. V. Iyengar (National Institute of Standards and Technology, U.S.), and K. Okamoto (National Institute of Environmental Studies, Japan). American Chemical Society: Washington, DC. 1991. xii + 363 pp. \$89.95. ISBN 0-8412-1888-9.

This book was developed from a symposium sponsored by the International Chemical Congress of Pacific Basin Societies in Honolulu during December 17–22, 1989. It consists of a preface, an introductory paper by lyengar titled The Need for Multidisciplinary Approaches in Biological Trace Element Research, and 27 papers in typescript form. These papers are grouped under the following sections: Planning Considerations; Quality Assurance; Determination; and Speciation and Bioavailability. There are indexes of authors, their affiliations, and subjects.

Pesticide Residues and Food Safety: A Harvest of Viewpoints. ACS Symposium Series 446. Edited by B. G. Tweedy (CIBA-GEIGY Corporation), Henry J. Dishburger (DowElanco), Larry G. Ballantine (Hazleton Wisconsin), and John McCarthy (National Agricultural Chemicals Association). American Chemical Society: Washington, DC. 1991. xv + 360 pp. \$59.95. ISBN 0-8412-1906-0.

This book was developed from a special conference sponsored by the Division of Agrochemicals of the American Chemical Society at Point Clear, Alabama, on January 21–25, 1990. It consists of a preface and 37 papers which are grouped under the following headings: Introduction, Pesticide Use: Where and Why; Alternative Agriculture Production; Exposure Assessment: Analytical Methods; Exposure Assessment: Residue Levels in Food; Risk Assessment; Risk Management; Legislative and Regulatory Issues; and Perspectives from the Media. There are indexes of authors, their affiliations, and subjects.

Books on Technological Chemistry

Absorbent Polymer Technology. Edited by Lisa Brannon-Peppas (Eli Lilly Research Laboratories) and Ronald S. Harland (KV Pharmaceutical Company). Elsevier Science Publishers: Amsterdam and New York. 1990. x + 278 pp. \$107.75. ISBN 0-444-88654-0.

This book is concerned with the consumer-oriented field of absorbent materials, the use of which in products for personal health care has grown greatly in recent years. Twelve contributed chapters are arranged in two sections: Fundamentals of Absorbent Materials (Preparation, Structure, Characterization), and Recent Experimental Studies. Thermodynamics, transport, swelling, structure, and performance are given attention. However, no explicit attention to the important problem of disposal is evident.

Saline Water Processing. Edited by Hans-Gunter Heitmann. VCH Publishers: New York. 1990. xx + 332 pp. \$98.00. ISBN 0-89573-871-6.

The members of a study group of The Water Chemistry Division of the German Chemical Society have contributed the 21 chapters in this book, which deals with all types of salt-containing waters, from natural sources to industrial wastes. The viewpoint is that of obtaining potable water or water for agricultural purposes; attention to pollution in the environment and its avoidance is much involved.

The chapters deal with such subjects as the following: sampling, analysis, and monitoring; colloidal aspects; scale formation; corrosion; flocculation and precipitation; reverse osmosis; ultrafiltration; ion exchange; electrodialysis; and the role of chlorine as a reagent and a product. The index is extensive.

Fire and Polymers. Hazards Identification and Prevention. ACS Symposium Series 425. Edited by Gordon L. Nelson (Florida Institute of Technology). American Chemical Society: Washington, D.C. 1990. xii + 627 pp. \$99.95. ISBN 0-8412-1779-3.

Polymers, which generally have a high carbon content, are inherently flammable, and because of the presence of other elements, they may emit a range of toxic materials when they burn. Wood, paper, and related materials are included along with synthetic polymers. In this volume of proceedings, fire toxicity, fire retardants and retardancy, thermal effects in combustion, and assessment and testing of fire risks are discussed in 34 typescript papers. The index is very thorough.

Additives for Water-Based Coatings. Special Publication No. 76. Edited by D. R. Karsa (Harcros Chemicals (UK) Limited). Royal Society of Chemistry: Cambridge. 1990. viii + 283 pp. \$91.00. ISBN 0-85186-607-7.

Ten typescript papers from a 1988 symposium organized by the Industrial Division of the Royal Society of Chemistry make up this softbound volume. The viewpoint in most of them is that of the formulator who is concerned with applications. The opening paper, "Additives for Water-based Coatings—A Polymer Chemist's View", by J. C. Padget, gives a review of the subject. The volume is well indexed.

Sounds and Vibration Damping with Polymers. ACS Symposium Series 424. Edited by Robert D. Corsaro (Naval Research Laboratory) and L. H. Sperling (Lehigh University). American Chemical Society: Washington, D.C. 1990. x + 469 pp. \$99.95. ISBN 0-8412-1778-5.

An ACS symposium held in Dallas in 1989 was the basis for the 25 typescript papers in this volume. Two of them are devoted to definitions and concepts. The others fall into the categories of dynamic evaluation, accoustic attenuation, polymeric materials, vibration damping, and advanced materials. The volume is well indexed.

Emerging Technologies in Hazardous Waste Management. ACS Symposium Series 422. Edited by D. William Tedder (Georgia Institute of Technology) and Frederick G. Pohland (University of Pittsburgh). American Chemical Society: Washington, D.C. 1990. xii + 402 pp. \$89.95. ISBN 0-8412-1747-5.

This book is about recycling, recovery of usable materials from wastes, and removal or destrution of contaminants, with particular emphasis on soil and water quality. There are 22 papers (reproduced from typescripts) including an introductory overview, "Emerging Technologies for Hazardous Waste Management", by D. W. Tedder and F. G. Pohland, all from a 1989 symposium held in Atlanta. Both organic and inorganic pollutants are considered. The subject index is thorough.

^{*} Unsigned book reviews are by the Book Review Editor.