Additions and Corrections

Chiral Pathways in the Thermal Rearrangement of 3,7-Dimethylene-1-ethyltricyclo[4.1.0.0^{2,4}]heptane to 2,5-Dimethylene-3-ethylbicyclo[4.1.0]hept-3-ene. Decyclization of a Pair of 2,2'-Linked Methylenecyclopropanes Avoids a Symmetrical 2,5-Dimethylenecyclohept-3-ene-1,6-diyl Biradical Intermediate [*J. Am. Chem. Soc.* **1991**, *113*, 4675]. MICHAEL D. WENDT and JEROME A. BERSON*

Page 4676: We thank Professor R. S. Sheridan for pointing out that the formal orbital symmetry designations for the pathways (1*S*,2*R*,4*S*,6*R*)-**1** to (1*R*,6*S*)-**2** and (1*S*,6*R*)-**2**, which are given in Scheme I as ($_\sigma 2_s$ + $_\sigma 2_a$), both should be ($_\sigma 2_s$ + $_\sigma 2_s$) instead. Accordingly, in the penultimate paragraph of text, the designation "allowed ($_\sigma 2_s$ + $_\sigma 2_a$)" should be "forbidden ($_\sigma 2_s$ + $_\sigma 2_s$)." In the last sentence of this paragraph, the word "antarafacially" should be replaced with "by double inversion". In the last sentence of footnote 13, "($_\sigma 2_s$ + $_\sigma 2_s$)" should be "($_\sigma 2_s$ + $_\sigma 2_a$)" and "forbidden" should be "allowed".

Computer Software Reviews

LOLI. Version 1.46. ChemAdvisor, Inc.: 13750 Merriman Road, Livonia, Michigan 48150. List price $3500.00 (with one group of lists as it is not sold separately; there are 4 groups of lists: Health, Environment, States, and International, each priced separately).

We live in a time of increasing government regulation. Nowhere is this trend more evident than in chemistry. The concerns that prompt these regulations include air and water pollution, toxic waste sites, worker safety, toxicological effects, transportation accidents, protection of citizens living near chemical industry, and safety of intermediate and consumer products. Numerous agencies at both state and federal levels of government are extensively involved in promulgating these regulations. Each agency has its own agendas, areas of concern, regulations, and inspection programs. The result is a bewildering array of over-lapping, isolated, and ever-changing sets of requirements that every chemical enterprise is expected to satisfy. Just keeping track of all these requirements is an enormous task.

The software tool LOLI, by ChemAdvisor Inc., is intended to provide some assistance to this task. It is a special information management program designed to maintain and use a database that exists in the form of multiple lists of chemicals. Each list might contain the chemicals falling under the scope of a particular regulating agency. Regulatory lists may be purchased from ChemAdvisor (and possibly other sources) or put in by the people using the LOLI program at the chemical site. ChemAdvisor has promised to continually upgrade each of their regulatory lists as the agencies responsible for them make changes and additions. Locally prepared lists might be useful for other in-house purposes, any place where information must be organized and used according to chemical substance.

LOLI is written for IBM compatible computers running MS-DOS or PC-DOS. A hard disk is required. The system is distributed on 3.5 or 5.25 in. disks. With all of the lists supplied by ChemAdvisor, the system requires about 5 MB of hard disk space. Another 3 to 5 MB might be needed as the system is used.

Compound Identification: The sorting and tracking mechanism used by the LOLI program is based on the Chemical Abstracts Service (CAS) registry number for each compound. Users can add non-official numbers for their own special purposes. The underlying strategy of operation is to first identify the CAS registry number for a compound of interest and then search one or more of the lists managed by this system to find that compound. There is a full set of tools for creating, maintaining, and searching these lists. All useful ways of viewing the data consistent with the way it is organized are provided.

The CAS registry number could be located off-line, such as using the printed or on-line versions of Chemical Abstracts or their indexes. Sometimes CAS registry numbers are included on container labels or in chemical catalogues. Usually a company will already know the CAS registry numbers of the compounds it regularly uses.

There is also a component in the LOLI program to find the CAS registry number from the common name or synonyms for the compound. It is called the CAS Table. This tool permits you to enter a full or partial name, specifying whether it is the start of the name or an embedded portion of it. An appropriate part of the CAS Table is displayed. From here you advance forward or backward until you find the compound you want. Once identified, you can carry the found CAS registry number into the other parts of LOLI to use as a search key. You can add your own synonyms for compounds in this table or put in new chemical species if they do not already exist. You can review an entry in this table to find all the synonyms listed for a given CAS registry number. There is a way to handle regulatory references of a nonspecific nature dealing with groups of chemicals or substances that are not unique compounds. When metals are regulated, it is often necessary to deal with the compounds in which they are found. The LOLI system provides for atom counts in these cases that allow the formula to be generated and percentages of each element to be obtained.

Using the Lists: Once the registry number of a compound is identified, a common activity would be to search all the lists to find the ones on which this compound appears. A report can be prepared giving the results of this search.

Often it is sufficient just to know whether or not the chemical is included in the regulatory scope of that agency. Other times you might also want to know additional information, such as legal discharge levels or toxicity limits. The LOLI program allows textual data of this type to be saved with the list entry, and it can be displayed once the compound is found during a search of the list. The LOLI program cannot search the chemical list using this data field as a search key. It can only show data that have been put into the list after the compound is located. Some of the regulatory lists provided by ChemAdvisor have supplementary information when it is pertinent. Users can add any information they wish to any list, including those they created themselves and those they purchased.

There are different ways one might want to utilize the information stored in these different lists. LOLI provides versatile tools for comparing lists and building new lists from existing ones. The logical operations AND, OR, EXCLUSIVE OR, and NOT can be used when combining existing lists. Once a new list is created, it can be used in subsequent combining operations. Virtually any kind of comparison or combination of lists is possible with these tools. The lists you create can be made permanent or left temporary so they erase when LOLI is finished. A

printing function lets you make hard copy of any lists or compound searches you have made. These lists can be put into a form acceptable to most of the common spreadsheet programs, which is a particularly valuable feature.

When you combine lists, only the data fields of one of them can be passed into the new list. This is a separate action the user must perform. In some cases, this restriction might be an important limitation of LOLI. Permanent lists can be edited to add data manually for any entry. The list editing function also allows you to change names of lists and add footnotes to explain exceptions or deal with other contingencies that do not fit anywhere else. You can add and delete compounds from the list. Sometimes when working with a list, you discover a need to revise the CAS Table containing registry numbers and chemical names. You might have a new compound or a new synonym to add. The list editing function permits you to also edit the CAS Table.

Maintaining the System: There are a set of utility functions that help you maintain the lists. They provide for merging purchased updates into lists and creating reports on what changes those update files will cause. You can off-load a list that can subsequently be reloaded on the same or a different LOLI system. This permits you to exchange your lists with others. You can create new lists from scratch or delete old lists no longer needed. There is a packing function that cleans up the disk files for better efficiency if data have been scattered by extensive editing of the lists.

The User Interface: The LOLI system has a reasonable look and feel. It follows a user interaction protocol quite similar to other software products with which chemists might be familiar. LOLI displays different screens at different points in the program and accepts commands and directions from the keyboard. Prompts for legal functions are shown on the screens. Highlights and color changes give the user good feedback.

The LOLI functions are easy to implement once one becomes familiar with the abbreviations and has basic understanding of the pathways that must be followed. Help screens are available and are reasonably clear. A chemist with some computer experience should be able to sit at the keyboard with the manual and learn how to operate the LOLI system in a few hours. This review was conducted on a ×286 machine running at 12 MHz. Response time was reasonable.

Conclusions: LOLI does not work like a typical relational database and would not be appropriate if searches are anticipated on the basis of some property other than the identity of the compound. It cannot manipulate the data entered for each compound, only display it. It cannot accept non-textual data.

LOLI is appropriate in those situations where keeping track of all the regulatory information is currently a problem. It is a useful tool for the people who must keep up with the regulations and be responsible for ensuring the organization meets its obligations. LOLI would be useful for other applications where the information is strictly list oriented. It is especially useful for dealing with multiple lists. For its intended niche, LOLI is a well-structured product that should serve its users well.

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Book Reviews

Structure and Dynamics of Bulk Polymers by NMR-Methods (NMR Basic Principles and Progress. Volume 21). By Vladimir D. Fedotov (USSR Academy of Sciences, Kazan) and Horst Schneider (Technische Hochschule Carl Schorlemmer Leuna-Merseberg, Germany). Edited by P. Diehl, E. Fluck, H. Günther, R. Kosfeld, and J. Seelig. Springer-Verlag: Berlin and New York. 1989. ix + 176 pp. $69.00. ISBN 3-540-50151 and 0-387-50151.

Despite the general nature of the underlying principles of magnetic resonance, its practice has become highly specialized. Some practitioners of NMR spectroscopy are so highly evolved that they are unable to communicate effectively with NMR experts in other fields, through lack of shared culture or, perhaps, temperament. This circumstance is partly a consequence of the inherent flexibility and richness of NMR spectroscopy: there is not a single, unique NMR experiment, but rather the NMR approach can be configured, under favorable circumstances, to address exactly *the* relevant question in many disparate scientific fields. Accordingly, the evolution of NMR spectroscopy in any particular field can be shaped by those with an insight into the fundamental scientific questions in that field. That is the approach taken by this most recent volume of the excellent *NMR Basic Principles and Progress* series. The authors write from positions of authority about the principles and techniques of magnetic resonance and, perhaps more importantly, about issues of polymer morphology and dynamical behavior.

This volume lays out the basic principles of magnetic resonance and moves almost immediately to a compendium of fundamental (pulsed) NMR methods which then see application throughout the book. Homonuclear methods are primarily emphasized, including determination of spin–spin and spin–lattice relaxation times in the laboratory and rotating frame; dipolar relaxation; and relaxation under pulsed spin-locking and under some simple homonuclear line-narrowing sequences. Other more specialized methods are discussed in a review format, with enough information to point the way into the primary literature. As the title of this volume indicates, the perspective is on polymer (physical) structure and dynamics. Little prominence is given to determination of chemical structure through the chemical shift spectrum: cross-polarization and magic angle spinning are discussed primarily for extracting relaxation rates.

Of particular interest is the insight which can be extracted from the free induction decay of the proton signal in polymers. At low temperatures the proton resonance in an organic polymer is quite broad, due to the diffuse magnetic dipolar couplings to other nearby protons; at higher temperature molecular motion modulates these couplings, narrowing the line and lengthening the spin–spin relaxation time T_2. While this phenomenon has been clearly understood in NMR spectroscopy for 40 years, there is no exact, closed-form expression describing how molecular motion reduces the dipolar couplings among many spins. Perhaps for this reason, detailed study of the temperature dependence of the T_2 relaxation time has not been popular recently. However, this book promotes the use and analysis of T_2 data, even by semiempirical relations, and one is impressed at the scope of information obtained.

This book is far more than a review. It presents the fundamentals of NMR spectroscopy, albeit tailored for polymer science, in a consistent fashion and integrates into this framework a detailed description of motions and morphology in organic polymers. A further benefit is that the authors draw heavily from their own work. Such work, especially the polymer studies of Dr. Fedotov, are less accessible to researchers who do not read the Russian scientific literature. Contributions of many other workers are presented clearly and with useful insight.

This book is to be commended, certainly to those with joint interests in NMR spectroscopy and polymers. Though not a primer of NMR spectroscopy, it is written from a sufficiently physical viewpoint that the polymer scientist with only a nodding familiarity with NMR spectroscopy may find some ideas in it. This volume may also prove useful to those interested in biopolymers and large protein structures, which share some features common to lightly cross-linked elastomers.

There are a few minor drawbacks in this volume. The book is most easily read cover to cover: the casual reader may find the search for important tables and equations rather tedious. Sometimes only written descriptions of complex phenomena are presented, with references back to the primary literature: here a key figure would have helped. The style of the figures is, to this reviewer, terse. On graphs, curves tend to be identified only by numbers: one must look into the caption or delve further into the text to determine the parameters associated with these numbers. Some light editing by the publisher would have made the English a bit smoother, though it is certainly readable, and the physical insight gained will more than repay the occasional extra wait for the verb.

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Nucleic Acids and Molecular Biology. Volume 4. Edited by Fritz Eckstein and David M. J. Lilley. Springer-Verlag: Heidelberg and New York. 1990. XII + 291 pp. $138.00. ISBN 0-387-52407-X.

This volume of the series is comprised of 17 chapters covering wide areas of Molecular Biology and written by recognized authorities in the field. The objective of this series is to publish focused review articles by active researchers. The reviews are not intended to be exhaustive, but rather to place the most recent data into context. This volume accurately represents this goal.

The first three chapters deal with unusual DNA structures and DNA binding to antitumor compounds and proteins. In Chapter 1, Frank-Kamentskii discussed the evidence supporting his proposed protonated triplex DNA structures for homopurine-homopyrimidine sequences at