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