Additions and Corrections

Generation and Characterization of Isomeric Iron–Silylene and Iron–Silene Cationic Complexes in the Gas Phase [*J. Am. Chem. Soc.* **1993**, *115*, 345]. R. BAKHTIAR, C. M. HOLZNAGEL, AND D. B. JACOBSON*

Page 346, second column, second sentence of the second full paragraph: The sentence should read "**1b** and **2b** both react with ethene-d_4 and ethene-$^{13}C_2$ to yield exclusive, initial adduct formation...". The sentence incorrectly listed complex "**1a**" instead of complex "**1b**".

Computer Software Reviews

MacSpec Version 1.0 and MassSpec Version 2.2. MacSpec—Spire Software: P.O. Box 1002, Maplewood, NJ 07040; (201) 762-0505. Written by Paul A. Zucker. List Price $295.00 for personal use and $250.00 for academic use. MassSpec—Trinity Software: P.O. Box 960, Campton, NY 03223; (800) 352-1282. Written by John Figueras. List price $95.00; Labpack (5 copies) $220.00.

MacSpec and MassSpec are mass spectra analysis programs designed for the Macintosh computer operation and are compatible with System 7. The MassSpec program and files are contained on a single 800K disk and require only 512 Kb of RAM for operation. The disk and the program may be run on the older Macintosh Plus units which are still in use at many university laboratory tutorial centers, and an MSDOS version is also available at the same price. MacSpec requires the Macintosh Plus or newer model with a system Version 6.0 and at least 1 Mb of Ram. The program and files are contained on two 800K disks; however, file searching procedures are improved when the program and files are copied to hard disk.

MassSpec Version 2.2 has incorporated several improvements over the earlier version (Version 1.0, 1989) with principal modifications to the structure drawing routines and a print option added to the file menu. The newer version can now be used in a multifinder mode. The structure graphics program is straightforward and easy to use for those familiar with other structure drawing routines. Conventional chemical structures can be entered, and the program will generate a database of fragments and then match structures in the database to the masses entered by the user. The user may select a mass peak from the mass listing, and the program will highlight those parts of the structure which correspond to the selected mass and provide isotopic M + 1 and M + 2 abundances. Structures containing up to 255 atoms and a molecular weight of 2417 or less may be used. Isotopic data are supplied to the program in an unformatted ASCII code and may be edited to provide mass data for specific mass spectrometers. MassSpec Files contain 40 representative chemical structures which serve as a tutorial guide for those learning the basics of structure fragmentation and mass spectroscopy. The user's manual and the program are clearly presented and will be the better choice for undergraduates and the novice who desire to learn just the basics of organic structural analysis by mass spectrometry.

MacSpec Version 1.0 is a newer and more sophisticated entry to the market. The user is provided a simple and versatile graphics program for structure entry. After the structure has been entered, the exact mass, percent elemental composition, and isotopic distribution for M + 1 and M + 2 are available from the window menu. From this point the program differs significantly from the application described above and offers a number of very useful tools to analyze spectral data and structural cracking patterns. The user may enter a suspected structure, select fragments from the structure, and determine the mass and isotopic peak patterns for each fragment. Entering a fragment mass or a peak selected from the spectrum, the user can generate a listing of possible formulas for the fragment based on the elemental composition of the starting structure. Various selective criteria can be used to limit the number of possibilities; however, an experienced chemist with moderate intuition can easily eliminate many absurd possibilities. Overlapping complex peak patterns due to two fragments of different elemental composition can be reconstructed and compared simultaneously on screen with the observed spectrum by the peak patterns or by percent peak abundances. The percent abundance of each fragment may be varied to achieve the matching pattern. Any portion of the spectrum may be enlarged to facilitate this comparison. Another feature offers analysis of "isotopic cluster"—that is, to determine a fragment formula from a fragment peak and its associated isotopic peaks using unit resolution mass spectral data. Peak pattern analysis for compounds containing deuterium, carbon-13, nitrogen-15, or oxygen-17/18 is achieved through a dialog box which enables the user to specify the percent isotope enrichment.

Metastable ions may be conveniently analyzed by entering up to 20 observed normal ion masses and then by entering the mass value for the metastable ion in question, the program determines whether the ion corresponds to a fragmentation pathway between any two of the normal ions listed.

After a fragment mass list (observed or user developed) has been created for a given structure, the "Losses" command produces a table crosslisting of all ions and their parent/product relationship. Selecting any entry in the table produces a window showing the structure, formula, and mass of the parent ion, the product ion, and the fragment lost.

A large 90-page manual and tutorial problems in the disc file directory facilitate getting acquainted with this versatile and somewhat complex program. Unfortunately, the manual frequently suffers from too many words and could be improved with a change in formatting and conciseness. The learning curve for MacSpec is a bit long; however, for the practicing chemist who has nontrivial mass spectrum analysis problems, the work is well worth the effort.

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