Additions and Corrections

Main-Group–Organotransition-Metal Chemistry: The Cyclopentadienylchromium Polyiodides Including $[(C_5Me_5)_2Cr_2I_3^+]_2[I_{16}^{2-}]$ [*J. Am. Chem. Soc.* **1990**, *112*, 1860–1864]. DAVID B. MORSE, THOMAS B. RAUCHFUSS,* and SCOTT R. WILSON

An important reference to previous work on organometallic polyiodides was omitted: Bottomley, F.; Darkwa, J.; Sutin, L.; White, P. S. *Organometallics* **1986**, *5*, 2165. The authors isolated $[(C_5Me_5)_2V(NO)]_2I_8$.

Computer Software Reviews

NMR″, Version 1.0. Calleo Scientific Software Publishers: 1300 Miramont Dr., Fort Collins, CO 80524. List price $275.00 for NMR″ and $375.00 for NMR″ II (faster Mac II or SE/30 version that requires a floating point coprocessor).

This program simulates NMR spectra, including second-order lines, from chemical shifts and coupling constants with use of Macintosh computers. The number of atoms that can be handled in one run, which depends on the currently available memory on your computer, is calculated and printed for you. All natural NMR-active isotopes of all elements are included, and dipolar as well as scalar coupling can be simulated. The program is very easy to use, at least for someone with experience on a Macintosh computer.

NMR″ requires a Mac 512KE, Mac Plus, Mac SE, or Mac II, with a Mac II or SE/30 recommended if simulating >5 $I = {}^1/_2$ spins. A six-spin test system that took several hours on an SE took only 9 min on a Mac II. Input consists of isotopes present (with user-defined abundances), chemical shifts, coupling constants, spectrometer frequency, line widths, spectrum width, tick mark spacing, and plot resolution. The output, a simulated spectrum, was comparable to that obtained with a different program with a larger computer in a test case.

NMR simulation programs with iteration routines (the user does the iterating with NMR″) are available with large spectrometers and externally for large computers, but in the former case it is necessary to tie up the instrument during the simulation, and in the latter case access to a large computer is needed. Thus, this small computer program has a place for academic or industrial users with appropriately configured Macintosh computers. It should be useful to students wishing to learn how the variation of chemical shifts and coupling constants affects NMR spectra and to researchers wanting to obtain the best shifts and coupling constants from the spectrum of a research compound.

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Book Reviews*

Sulphur-containing Drugs and Related Organic Compounds. Chemistry, Biochemistry and Toxicology. Volume 1: Part A. Metabolism of Sulphur Functional Groups. Edited by L. A. Damani (Kings College London, University of London). John Wiley & Sons: Chichester and New York. 1989. 167 pp. $89.95. ISBN 0-470-21257-8.

Volume 1, Part A, begins a projected three-volume series, each volume to be in two parts. The series will emphasize the chemistry and biochemistry of biotransformations and drug toxicity of sulfur-containing xenobiotics, i.e., compounds acquired from the environment by living organisms (in quotations, **ph**, the British style for sul**ph**ur, will be used for the American style of **f**). The Editor states that "until now a comprehensive compilation of metabolic and toxicological data on sulphur compounds has not been published". The readership claimed includes biochemical, clinical and other types of pharmacologists, toxicologists, biochemists, organic and medicinal chemists, and "medical scientists".

The 167 pages by eight coauthors include the following seven chapters: general organic chemistry and biochemistry of sulphur (20 pages, 51 refs); natural occurrence (32 pages, 127 refs); agricultural chemicals (32 pages, 99 refs); other industrial and medicinal aspects (19 pages, 29 refs); inorganics (22 pages, 108 refs); and the functionalities of thioethers, thiols, dithioic acids, and disulphides, first as to oxidation, reduction, and hydrolysis (16 pages, 47 refs) and then as to biochemical conjugations (10 pages, 37 refs). Although the authors "were asked to ensure that the coverage of material was comprehensive", the total of only about 500 references for the breadth of topics covered seems a bit sparse; for example, Jocelyn's *Biochemistry of the SH Group* alone contains 2000

*Unsigned book reviews are by the Book Review Editor.