COMPUTER SOFTWARE REVIEWS

LAOCOON. An NMR Simulation Program

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Several years ago, a second-order NMR simulation program, RACCOON, was written by Paul F. Schatz, of the University of Wisconsin—Madison. More recently, another similar program called LAOCOON PC NMR Simulation has appeared. LAOCOON[1] was written by Joseph S. Thresher, Department of Chemistry, University of Alabama—Tuscaloosa.

Both programs are capable of calculating the NMR spectra of two to seven spin one-half nuclei given their shifts and coupling constants. The units of the chemical shifts can be in either ppm or Hz. The coupling constants must be in Hz, but the spectrometer frequency may be given in MHz. LAOCOON features the calculation of positions of up to 300 lines. It can also provide lists of spectral lines, intensities, and line widths.

The program has a main Menu on the screen which is very easy to follow and use. Most of the calculations can be done within 3 min. It is a valuable tool in teaching the second-order NMR concept. It can also be very helpful in research. The chemical shifts in a second-order NMR are field dependent. When the magnitude of the separation between two peaks in the NMR, expressed in Hz, is of the same order of magnitude as the coupling constant, second-order spectra are produced. The best illustration in teaching such a concept is to analyze and calculate a sample spectrum with the simulation program. We have experienced the application of the program in our research where we tried to prepare a known[2] nickel phosphorus complex, $Ni(CH_2PPh_2CHPPh_2)_2$. The $^{31}P\{^1H\}$ NMR spectrum we obtained from a 200 MHz NMR spectrometer was different from the reported spectrum in chemical shifts, coupling constants, and line widths.[3] The reported paper did not mention the frequency of the spectrum recorded. After analysis and calculation with the simulation program, the complex we prepared was shown to be the same as that reported in that paper.

Both RACCOON and LAOCOON simulation programs require an IBM PC, XT, AT or compatible computer with at least 384K memory, one disk drive, and an IBM compatible color graphics adapter with an EGA adapter. The programs require DOS 2.00 or higher be used. The HP 7475 plotter or a graphics printer can be supported for graphics output. Our experience with the program in teaching and research has been excellent. J. Gong acknowledges Research Corporation for Cottrell College Science Award, and S. Hinze thanks NASA JOVE Scholarship.

REFERENCES AND NOTES

(1) LAOCOON is available from Dr. Joseph S. Thresher, Department of Chemistry, University of Alabama—Tuscaloosa at a cost of $75.00.

(2) Gong, J. K., Peters, T. B., Fanwick, P. E., Kubiaak, C. P. *Organometallics* **1992**, *11*, 1393.

(3) Schmidbaur, H., Deschler, U., Milewski-Mahrla, B. *Angew. Chem., Int. Ed. Engl.* **1981**, *20*, 586.

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