gNMR version 3 for Macintosh

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gNMR is an NMR spectral simulation package capable of simulating spectra for systems containing nuclei with spins up to 9/2. The effective system size limit is 10 magnetically inequivalent nuclei simply due to program speed. The user's manual contains a very useful tutorial chapter, which provides an overview of the features of the program with sample data to work with. The program can simulate simple spectra or can be used to iteratively match an observed spectra. These two abilities make the program useful from both an educational and a research perspective.

A molecule for spectral simulation can be entered in two modes. A structure can be imported from a file produced by ChemDraw or Chemintosh, and the program can estimate chemical shifts and coupling constants for the nuclei in that molecule. Alternatively, the numbers of magnetically equivalent nuclei, their chemical shifts, and their coupling constants can be entered manually. This mode is most useful for determining parameter values by providing an initial guess that can be optimized by either full lineshape iteration or assignment iteration against an experimental spectrum.

Installation of gNMR is very straightforward. The installer program determines whether to install the FPU or non-FPU version and prompts for necessary disks. A standard installation is available, or the installation can be customized. The installation disks provide a useful set of notes, examples, and tutorial files

Educational Benefits. The 'import structure' option allowed students to easily explore the three components of an NMR spectrum that are most commonly emphasized in a sophomore organic chemistry class. Simple comparison of the simulated spectrum of methane to methyl bromide demonstrated the effect of electronegative atoms on the observed chemical shift. Methyl bromoacetate provided a clear example of the relationship between relative signal areas and ratios of protons contributing. Bromoethane demonstrated a simple case of spin−spin splitting. Student response indicated that this would be a useful learning tool for those who learn best through "hands-on" type activities.

Research Benefits. Although gNMR does a very good job of 'guesstimating' parameters for simple systems, a molecule such as threose is not easily simulated by a one-pass simulation. Simulation of more complicated spectra requires either a detailed understanding of the spin systems and chemical shifts involved or an experimental spectrum to iterate against. Using gNMR as a research tool will entail a great deal more work than simply using it as an educational tool. It does have a number of capabilities including chemical-exchange calculations, optimization of peudo-first-order rate constants, use of symmetry, and approximate calculations that make gNMR a very flexible tool.

Minimum System Requirements. These are the minimum system requirements: an MC68020 or higher CPU, an MC68881 (or higher) math coprocessor,[1] system 6.0.5, 4 Mb of memory, and 5 Mb of free space.

REFERENCES AND NOTES

(1) A non-FPU version is available but is considerably slower.

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