

"Student-Determined Values for the Calculation of Chemical Shifts of Methylene Protons in Different Chemical Environments." Breton, G. W. *Journal of Chemical Education*, 2000, 77, 81-83.

Abstract: Nuclear magnetic resonance (NMR) spectroscopy has gained a place of preeminence in chemistry among methods of molecular structure determination (1-3). Its use is prevalent in both academic (i.e., graduate schools) and industrial settings. It is therefore vitally important that undergraduate chemistry majors be familiar with the basic experimental techniques and spectral interpretive skills associated with NMR spectroscopy.

We introduce  $^1\text{H}$  NMR spectroscopy in the first semester of our organic chemistry course in conjunction with the relevant chapter from the textbook. An elementary (and brief) discussion of the theory of instrument operation is followed by an in-depth discussion on the topics of chemical environment, chemical shift, and spin-spin coupling. The concept of chemical shift is reinforced by the introduction of a table (see Table 1) that allows for the rapid calculation of approximate chemical shifts for methyl, methylene, and methine protons in a variety of common chemical environments. Similar tables are readily available in the literature (4-6). Since this is an introduction to  $^1\text{H}$  NMR spectroscopy, we focus primarily on simple organic compounds with single functional groups and generally consider only the effect of  $\alpha$ -substituents on chemical shift. (Even with this approximation, most calculations using the data in Table 1 are reliable to within 0.5 ppm.) We have found that the students are quite amazed at how easy it is to calculate the predicted chemical shift of any given proton environment using the table.

We desired an experiment for the associated laboratory course (which we try to run conceptually "parallel" to lecture) that would demonstrate the effect of different commonly encountered chemical environments on chemical shift. We found, however, that with few exceptions (7-10), most widely used laboratory texts and many introductory experiments from this *Journal* (11-13) tend to introduce  $^1\text{H}$  NMR spectroscopy as a means of analysis for products derived from a reaction.<sup>1</sup> The student's initial use of  $^1\text{H}$  NMR spectroscopy, therefore, is relegated to secondary importance in an otherwise unrelated experiment that constitutes the primary focus of the lab exercise. We concluded that a new experiment was in order that had as its *primary* focus the operation of the NMR spectrometer and interpretation of representative spectra. Furthermore, we decided that it would be instructive for the students to construct a table for the calculation of chemical shifts – such as the one used in the lecture portion of the class (i.e., Table 1) – using spectral data obtained on their own.