Title of departmental seminar

Teaching NMR Spectroscopy Concepts Using Specifically Deuterated Molecules

Abstract summary of seminar

Nuclear magnetic resonance (NMR) spectroscopy is taught in most every majors-level organic chemistry course, specifically as an analytical technique used to determine the structure of small organic molecules. This approach sets a foundation for advanced courses, where structural studies of larger molecules (including polymers and biomolecules) are considered or reaction parameters (kinetics and thermodynamics) are evaluated. In addition, there are experiments suited for first-year students designed to introduce the technique and for non-majors courses designed to draw parallels to magnetic resonance imaging. Such a rich trove of creative laboratory experiments and classroom materials allows faculty to design a scaffolded curriculum specific to the needs of a degree program, a track or specialization, or even an individual student. Modern Fourier transform NMR spectroscopy relies on the use of deuterated solvents (that may also be analyzed using continuous wave techniques) yet the utility of analyzing specifically deuterated molecules receives much less attention in the curriculum. Specific deuteration may be introduced in organic chemistry and more examples are found in advanced courses where deuterium plays a key role in the determination of chemical mechanisms. In this presentation, I explore the usefulness of specifically deuterated molecules as teaching tools for the interpretation of NMR spectra. Accurate interpretation of NMR spectra relies on concepts of chemical shift, integration, and spin-spin splitting. Student understanding of these concepts are challenged when they compare and contrast NMR spectra from a series of isotopologues ("isotopic homologues"). Of course, instructors do not want to overwhelm students with arcane or superfluous examples! The examples included here are weaved into common reactions universally taught in the organic chemistry curriculum. Thus, the introduction of specifically deuterated molecules allows student to (a) solve a problem of spectral interpretation; (b) reinforce foundational concepts in NMR spectroscopy; and (c) scaffold their learning objectives from organic chemistry into advanced courses in chemistry and biochemistry.