CH-314 Structural Analysis
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Jigsaw 1E

Introduction to Nuclear Magnetic Resonance

1. [Keeler Section 2.1] In a ^{1}H NMR spectrum measured in a 400 MHz spectrometer, the peak from TMS (the reference compound) is found to occur at 400.130000 MHz. Two other peaks in the spectrum are found at 400.135023 and 400.137921 MHz.

    a. Compute the chemical shifts of these two peaks in ppm.

    b. This sample is re-run on a different spectrometer which operates at 900 MHz for protons. The reference frequency for this spectrometer is 900.130000 MHz. What would be the frequency, in MHz and ppm, of the other two peaks on this spectrometer?

    c. Why do we generally report peak locations in ppm?

    d. [Keeler Section 2.5] What would the frequency separation, in Hz and in $rad \cdot s^{-1}$, be between these two peaks on the 400 MHz and 900 MHz spectrometers?

    e. Based on this, is it worth it using higher magnetic fields? Why? *See also: Jigsaw 1D.2*

2. [From Past Exam] Consider 3 spins, A, B and C. The chemical shift of A is 120 Hz, and J_{AB} = 12 Hz, J_{AC} = 4 Hz, J_{BC} = 6 Hz. (The chemical shifts of B and C are 1000 and 2000 Hz respectively). *See also: Jigsaw 1A.1*

    a. [Keeler Section 2.3] Draw the multiplet pattern that would be seen for spin A.

    b. [Keeler Sections 2.3 and 3.6] Label the frequencies, intensities, and spin states of each peak in the multiplet pattern.

    c. [Keeler Section 2.1] Calculate the separation between peaks in ppm for a 400.130000 MHz spectrometer and a 900.13000 MHz spectrometer.

    d. Repeat step (a) for J_{AB} = 10 Hz and J_{AC} = 10 Hz. What special feature arises when $J_{AB} = J_{AC}$?