

## Jigsaw 1A

### Keeler Section 2.1. NMR frequencies and chemical shifts

In a  $^1\text{H}$  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 400.131023 and 400.132179 MHz.

1. Compute the chemical shifts of these two peaks in ppm.
2. This sample is re-run on a different spectrometer which operates at 600 MHz for protons. The reference frequency for this spectrometer is 600.130000 MHz. What would be the frequency, in MHz and ppm, of the other two peaks on this spectrometer?
3. Why do we generally report peak locations in ppm?
4. Based on part (2), is it worth it using higher magnetic fields? Why?
5. What's one reason there are a wide range of magnetic fields used in modern spectrometers? (i.e., why don't we all just use the "best" one?) Hint: Think about the Build-A-Spectrometer activity from earlier.