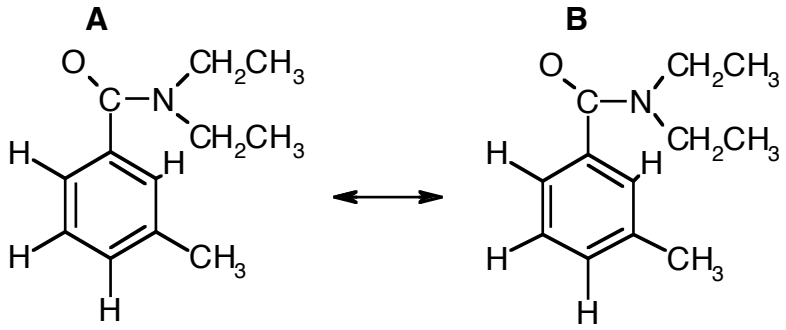
Name(s): _____ *Sec.* _____
Chem 227/ Dr. Rusay

Postlab : Synthesis of DEET

NMR: Resonance/ Rotations/ Conformations

1. Using the *NMRs* that were provided. Consider the ^{1}H *NMR* data and which protons are chemically equivalent. Complete the two DEET resonance structures shown below, which will be used to explain the *NMR*. Number the chemically equivalent protons in the structures, predict the theoretical signal splitting, and assign the peaks in the spectrum to their chemical shifts in the table below.

A ⟷ **B**



^{1}H (ppm)	peak splitting	peak assignment #

2. What are the relative percentages of **A** and **B** for the two respective resonance forms in the NMR mixture? Show your calculation and briefly explain your reasoning.

3. If the ^{1}H spectrum were recorded at high temperature, the two pairs of signals (4 total) would collapse into two separate signals. Calculate the respective chemical shifts for the chemically equivalent protons of the ethyl groups at high temperature. (Note: the spectrum was recorded using a 300Mhz instrument.)

4. If the proton spectra (high temperature and low temperature) were recorded on DVC's 60 MHz NMR, what would be the expected change in the *NMR?* Briefly describe your reasoning assume that the chemical shifts from the low temperature 300 MHz *NMR* would be the same in the case of the 60 MHz spectrum.

5. Consider only the ethyl groups in the ^{13}C NMR. Is the same conformational/rotational NMR phenomena observed as in the ^{1}H NMR? Provide a detailed explanation citing chemical shift data from the ^{13}C NMR for your answer.