Chem 625 Return to Modern NMR

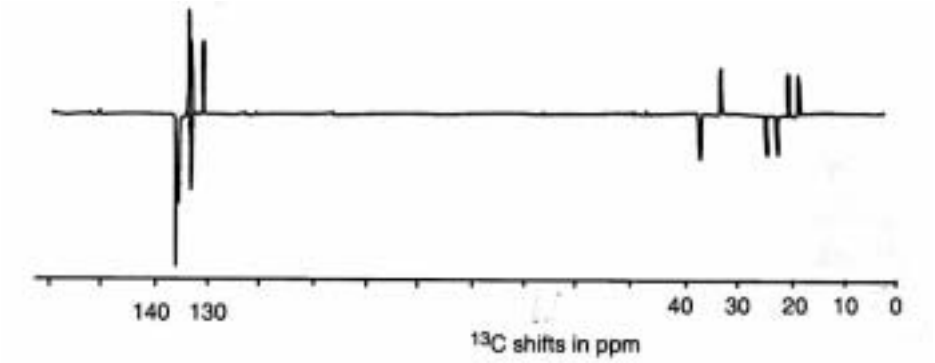
Professor Zax April 19, 2002

These problems should be turned in by Friday, April 26.

1. Consider an experiment in ^{13}C NMR where TMS (defined to have a shift of 0 ppm) appears at 100.000000 MHz, precisely. We choose 100.000000 MHz as our resonance frequency, establish a sampling rate of 20 kHz, and run an experiment. At what frequency (in kHz), or at what shift (in ppm), do we observe a carbonyl peak with chemical shift 180 ppm?

2. We are working in a large magnetic field where the ^{1}H resonance frequency of TMS is exactly 400.000000 MHz (which establishes our chemical shift scale, as the shift of TMS is defined to be 0 ppm). Assume that we wish to observe a "normal" ^{1}H NMR spectrum, with a little room to spare, so we will require a data "window" covering 15 ppm, from –2.5 to +12.5 ppm. We also expect some small *J* couplings, and will therefore require that (without zero filling!) the digital resolution is no worse than 0.25 Hz/point. Choose a resonance frequency (center frequency), sampling rate (or, equivalently, the time between sampled points), and a total number of data points which will satisfy these conditions.

3. Consider the ordinary INEPT spectrum illustrated below, observed in a compound of chemical formula C_8H_{10}. Write a structure consistent with the spectrum, and explain your reasoning.



4. Imagine that your boss unreasonably insisted on observing quaternary C sites in his (her) ^{13}C NMR spectrum, yet still required that the experiments be carried out using "modern" methods of polarization transfer so as to save his (her) research funds for a group dinner. He (she) suggests using long-range $^{2}J_{C\text{-}H}$ couplings (typically 1-2 Hz) to enhance the otherwise missing ^{13}C signals via INEPT. Argue for (or against) his suggestion; i.e. either design the experiment if you think it should work, or suggest what the problems might be in getting it to work if you think he (she) has lost his (her) senses.