NAME:

Section:

## CHE 311L Spectroscopy Problems

1. Using the on-line NMR spectra for the Nitration of Methyl Benzoate experiment, draw the structure of the starting material, methyl benzoate, directly on its <sup>1</sup>H NMR spectrum with all non-equivalent H's labeled (a,b,c...) for NMR identification. Match each label with the corresponding peak(s) in the spectrum by writing the appropriate letter above the associated peak(s). Label any NMR solvent peaks in the spectrum by writing the solvent above them. Only turn in the one spectrum that shows all of the peaks.

Draw the structure of the product, methyl m-nitrobenzoate, directly on its <sup>1</sup>H NMR spectrum with all non-equivalent H's labeled (a,b,c...) for NMR identification. Match each label with the corresponding peak(s) in the spectrum by writing the appropriate letter above the associated peak(s). Label any NMR solvent peaks in the spectrum by writing the solvent above them.

Fill out the table below for the <sup>1</sup>H NMR spectrum of the product, methyl m-nitrobenzoate. Use the same labels (a,b,c...) in the table that were used for identification of non-equivalent protons on the spectrum. You may use the expanded spectrum to determine chemical shifts and coupling constants, but you will only turn in the one spectrum that includes all the peaks. Do not include solvent peaks in the table. See the Introduction to NMR experiment from CHE 310 to see how an NMR table is correctly filled out.

<sup>1</sup>H NMR spectrum of the product

δ (ppm)	Multiplicity	J, Hz	Number of H's	Identification

Show one example each of a chemical shift and coupling constant calculation.

2. You are given four samples, containing one compound from each pair below. For each sample you can use only one spectroscopic technique, <sup>13</sup>C NMR, IR, UV-Vis, MS (not exact mass) or optical rotation to examine it. Furthermore, each technique may only be used once. Which technique would you use for each of your samples? Briefly explain your answers stating specifically what you would observe that would allow the two compounds to be distinguished.

