¹H NMR Spectroscopy

Problem Set 3 CHEM 393 Dr. H.M. Muchall

- 1. The following ¹H NMR spectrum was recorded on a 60 MHz spectrometer. It shows three signals. The molar mass of the hydrocarbon is 120 g/mol.
 - a) (1 point) What causes the unidentified, unintegrated signal?
 - b) (1 point) What are the chemical shifts of signals a and b in ppm?
 - c) (4 points) Which compound is it?
 - d) (3 points) Calculate the chemical shift for all non-equivalent protons.

e) (2 points) Give a closely related isomeric compound and reason why it is not a proper solution.

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- 2. Predict the ¹H NMR spectra for the following compounds. Include chemical shift (with evaluation), integration and multiplicity. Give proper drawings that consider the intensity of the lines within a multiplet.
 - a) (4 points)

b) (5 points)

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- 3. For each set of ¹H NMR data, suggest a structure that is consistent with the data.
 - a) (2 points) C₃H₅Cl₃: 2.20 ppm, 3H; 4.02 ppm, 2H
 - b) (2 points) C₇H₈O: 2.43 ppm, 1H; 4.58 ppm, 2H; 7.28 ppm, 5H



4. (11 points) Two isomeric ketones show the following ¹H NMR spectra. Identify the compounds. Provide full labels for all signals.

5. (8 points) The following multiplets are due to protons A, M and X. Determine the signal multiplicity, the coupling constants J_{AM} , J_{AX} and J_{MX} as well as the number of protons in each group (take the sum of the height of the lines as an integral). Classify the systems as AMX or AM_2X .



6. (10 points) Identify the compound that shows the following ¹H NMR spectrum. Provide full labels for all signals.

