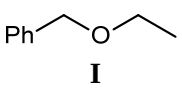
CHEM 393
Sample "Midterm" Exam
Dr. H.M. Muchall

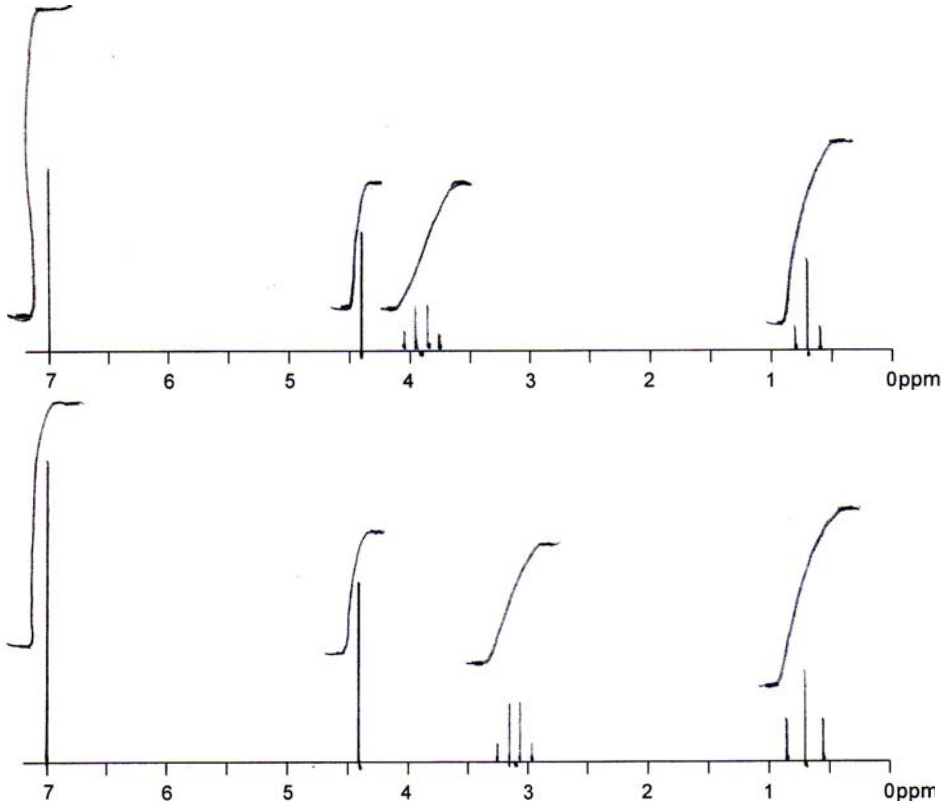
Name _____

Remember: about a point a minute! This exam would be set for 60 minutes.

1. Students were instructed to draw, accurately, the 60 MHz ^{1}H NMR line spectrum of **I** using a ^{3}J of 6 Hz. The following are two of their replies.



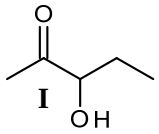
I



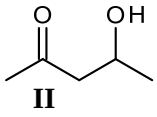
a) (7 points) List multiplicity, integration and calculated chemical shift for each set of protons in **I**. Briefly evaluate each calculated chemical shift for accuracy. Treat the phenyl protons as "s, 5H, 7.0 ppm".

b) (3.5 points) On the spectra above, and following from a), point out all the shortcomings in the student replies.

2. Distinguish between compounds using their ^{13}C NMR spectra.



I

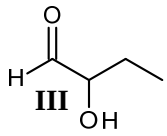


II

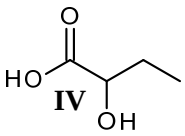
a) (4 points) For **I** and **II**, list the multiplicity for each signal in a proton-coupled spectrum. Does this allow a distinction between the compounds?

b) (4 points) For **I** and **II**, list the chemical shift (calculate using tables A8.2 and A8.3) for each methyl signal. Briefly evaluate each calculated chemical shift for accuracy. Does this allow a distinction between the compounds?

c) (2 points) Comment on why/how you can use the carbonyl signal to distinguish easily between **I** and **III** and between **I** and **IV**.

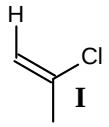


III

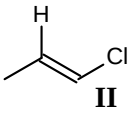


IV

3. For alkenes **I** and **II**,



I



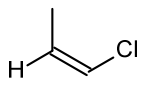
II

a) (3 points) give the multiplicity of each ^{1}H signal (if you cannot decide just from the structure, give both options).

b) (2 points) for the two identified protons only, give their coupling(s) as ^{2}J, ^{3}J and/or ^{4}J.

c) (4 points) from b) and tables A14, accurately draw the two tree diagrams using 10 Hz per cm (use a ruler!). Clearly state the J values you are using on the diagrams. (Now the answer to a) should be clear!)

d) (2 points) from c), how would the signal/tree diagram for the indicated proton in **III** differ from that in **II**?



III

4. Circle ***all*** that apply. Conflicting answers for a question will lose you all points for that question.

I. (2 points) The terms ‘upfield’ and ‘downfield’
a) refer to relative signal positions.
b) refer to absolute signal positions.
c) refer to the relative height of the signals.
d) are often used to compare chemical shifts.

II. (2 points) The Boltzmann distribution for protons at equilibrium
a) depends on the magnetic field strength.
b) does not depend much on the temperature.
c) gives an overpopulation of the +1/2 spin on the order of tens to hundreds per million.
d) gives an overpopulation of the –1/2 spin on the order of tens to hundreds per million.

5. (5 points) Circle TRUE or FALSE for the following statements.

a) FT-NMR spectrometers record an emission signal rather than an absorption signal. TRUE/FALSE

b) The resonance condition implies that a proton with ω of 60 Hz requires a detection frequency of 60 MHz. TRUE/FALSE

c) Under special circumstances only, CH_3OH is an AX_3 spin system. TRUE/FALSE

d) At a given magnetic field strength, γ of the nucleus determines ω. TRUE/FALSE

e) For a given nucleus, the magnetic field strength determines ω. TRUE/FALSE