CH0310, ORGANIC CHEMISTRY I
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Quiz 10, Take home, due midnight ***Saturday***, March 28, 2009

Submit the quiz in pen, or Xerox/fax/scan your pencil copy

Hand in before/after class on Friday
Drop off at 1101 CSC (before 5 pm Friday)
Fax to 412-624-9861 (till midnight Saturday)
Email to lynnec@pitt.edu (till midnight Saturday, ***pdf file only!***)

Interpretation of ^{13}C and ^{1}H NMR Spectra

To prepare:

- read Chapter 10, focusing on Sections 10.4-10.9
- review lecture notes for March 23 and 25
- Do problems 25-41 in Chapter 10

You need to know how to assign structures for simple molecules if given a molecular formula and an NMR spectrum. You need to be able to interpret spectra by assigning resonances to nuclei in a molecule based on chemical shift, integration, and spin-spin coupling.

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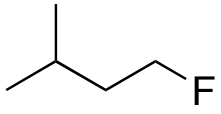
NAME SIGNATURE

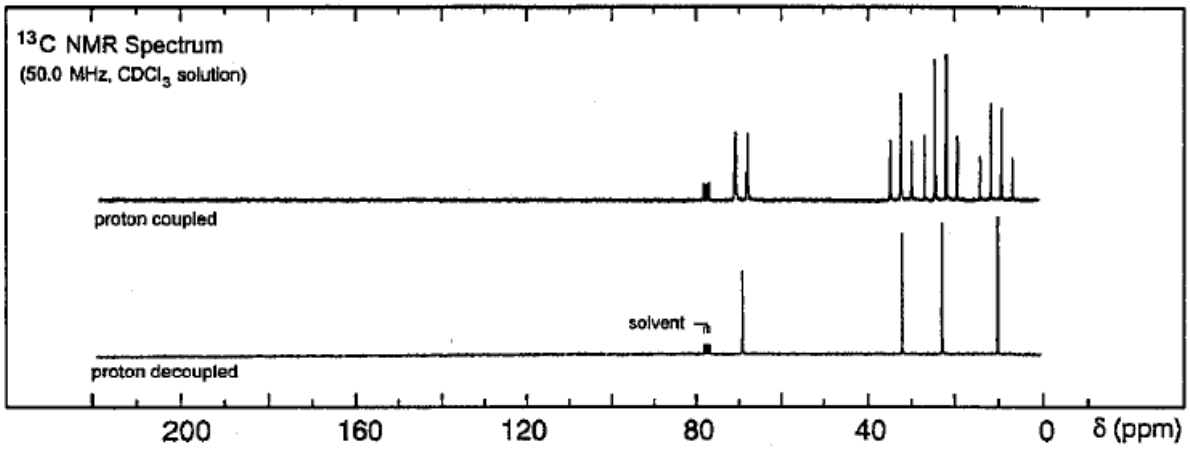
Interpretation of ^{13}C and ^{1}H NMR Spectra

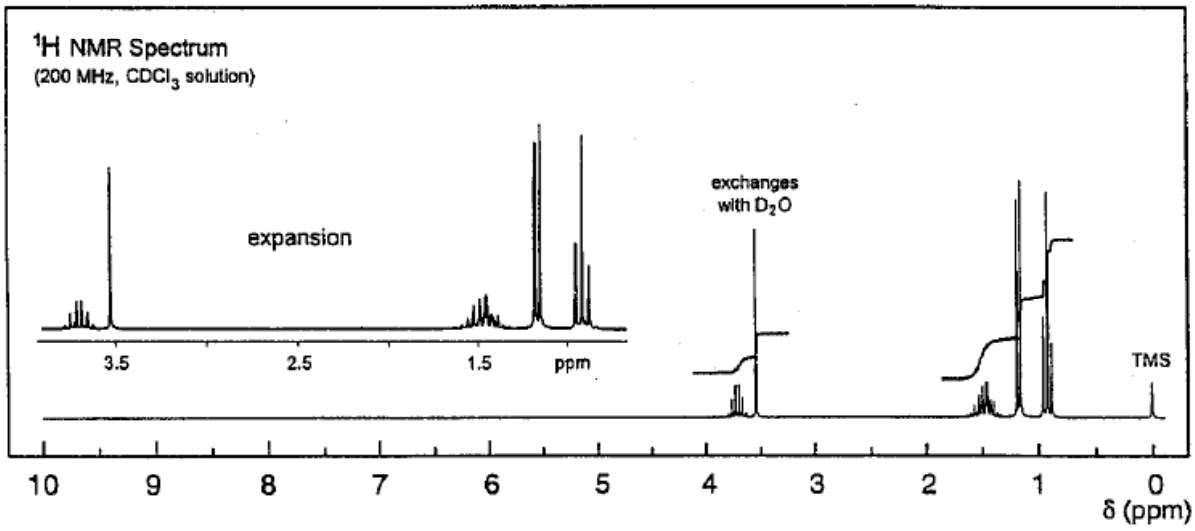
1) Assign all the resonances for the ^{1}H and ^{13}C NMR spectra of the following compound and explain how you made each assignment (3 points).
^{1}H NMR spectrum: δ 4.10 (t, 2 H), 1.83 (m, 1 H), 1.45 (q, 2 H), 1.01 (d, 6 H).
^{13}C NMR spectrum: δ 81, 40, 25, 22.



2) An ***isomer*** of the compound in (1) exhibits the following spectra. Show the structure and explain how you assigned it from the data (3 points).
^{1}H NMR spectrum: δ 1.45 (q, 2 H), 1.40 (s, 6 H), 0.96 (t, 3 H).
^{13}C NMR spectrum: δ 94, 37, 28, 4.

3) On the next page are ^{1}H and ^{13}C NMR spectra of an unknown: $C_4H_{10}O$. What is its structure and how did you decide? (4 points)


^{13}C NMR Spectrum
(50.0 MHz, $CDCl_3$ solution)
proton coupled
solvent
proton decoupled
200
160
120
80
40
0
δ (ppm)


^{1}H NMR Spectrum
(200 MHz, $CDCl_3$ solution)
expansion
3.5
2.5
1.5
ppm
exchanges
with D_2O
TMS
10
9
8
7
6
5
4
3
2
1
0
δ (ppm)