CHEM 8M $^1$H NMR Problems (McMurry, Organic Chemistry, 8$^{th}$ Edition)

#14 – 18 = 5 pts toward Exp 2 pre-lab, day 2

**Problem 13.14**
How many kinds of electronically nonequivalent protons are present in each of the following compounds, and thus how many NMR absorptions might you expect in each?

(a) CH$_3$CH$_2$Br  
(b) CH$_3$OCH$_2$CH(CH$_3$)$_2$  
(c) CH$_3$CH$_2$CH$_2$NO$_2$  
(d) Methylbenzene  
(e) 2-Methyl-1-butene  
(f) cis-3-Hexene

**Problem 13.16**
Each of the following compounds has a single $^1$H NMR peak. Approximately where would you expect each compound to absorb?

(a) \[ \text{ } \]
(b) \[ \text{ } \]
(c) \[ \text{ } \]

(d) CH$_2$Cl$_2$  
(e) \[ \text{ } \]
(f) \[ \text{ } \]

**Problem 13.17**
Identify the different kinds of nonequivalent protons in the following molecule, and tell where you would expect each to absorb:

\[ \text{ } \]

**Problem 13.18**
How many peaks would you expect in the $^1$H NMR spectrum of 1,4-dimethylbenzene (para-xylene, or $p$-xylene)? What ratio of peak areas would you expect on integration of the spectrum? Refer to Table 13.3 for approximate chemical shifts, and sketch what the spectrum would look like. (Remember from Section 2.4 that aromatic rings have two resonance forms.)

\[ \text{ } \]
Spin-Splitting in $^1$H NMR Spectra

To interpret the NMR information, let's look at each absorption individually. The three-proton absorption at 0.92/4 is due to a methyl group in an alkane-like environment, and the triplet splitting pattern implies that the CH$_3$ is next to a CH$_2$. Thus, our molecule contains an ethyl group, CH$_3$CH$_2$.

The six-proton singlet at 1.20/4 is due to two equivalent alkane-like methyl groups attached to a carbon with no hydrogens, (CH$_3$)$_2$C, and the two-proton quartet at 1.50/4 is due to the CH$_2$ of the ethyl group. All 5 carbon and 11 of the 12 hydrogens in the molecule are now accounted for. The remaining hydrogen, which appears as a broad one-proton singlet at 1.64/4, is probably due to an OH group, since there is no other way to account for it.

Putting the pieces together gives the structure: 2-methyl-2-butanol.

**Problem 13.19**
Predict the splitting patterns you would expect for each proton in the following molecules:
(a) CHBr$_2$CH$_3$
(b) CH$_3$OCH$_2$CH$_2$Br
(c) ClCH$_2$CH$_2$Cl
(d) CH$_3$CH$_2$COCH$_2$CH$_3$
(e) CH$_3$CH$_2$COCH$_3$
(f)CH$_3$

**Problem 13.20**
Draw structures for compounds that meet the following descriptions:
(a) C$_2$H$_6$O; one singlet
(b) C$_3$H$_7$Cl; one doublet and one septet
(c) C$_4$H$_8$Cl$_2$O; two triplets
(d) C$_4$H$_8$O$_2$; one singlet, one triplet, and one quartet

**Problem 13.21**
The integrated $^1$H NMR spectrum of a compound of formula C$_4$H$_{10}$O is shown in Figure 13.17. Propose a structure.

**Figure 13.17** An integrated $^1$H NMR spectrum for Problem 13.21.
** Pay attention to “Chem Shift” and “Rel. area” table to determine number of peaks and relative integration values (number of H’s per signal).

21.70 Assign structures to compounds with the following \(^1\)H NMR spectra:

(a) \(\text{C}_5\text{H}_{10}\text{O}_2\)

IR: 1735 cm\(^{-1}\)

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(b) \(\text{C}_{11}\text{H}_{12}\text{O}_2\)

IR: 1710 cm\(^{-1}\)

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