Chemistry 333  
Organic Lab Lecture 

Name: Key 

Exam #1 

This is an open-book, open notes exam. Show your work, so you can receive credit for correct parts of the final molecule. 

1. (20 points) \( \text{C}_4\text{H}_9\text{Br} \) \( \text{IHD} = 0 \) 
  
\[
\begin{align*}
42.5, \text{t} \\
30.7, \text{d} \\
21.0, \text{q (2)} \\
\end{align*}
\]

\( \text{H}_3\text{C} \) symmetry 

\( \text{H}_3\text{C} \) 

One branch point, so three end groups. Two are methyls, the other must be \( \text{CH}_2\text{Br} \). 

\[
\begin{align*}
\text{Br} \\
\end{align*}
\]
2. (40 points) \[ \text{C}_8\text{H}_{16}\text{O} \]

\[ \text{IHD} = 1 \]

There are 15 H's attached to C, so one must be attached to O

\[ \begin{align*}
141.4, \text{ d} \\
114.4, \text{ t} \\
73.2, \text{ d} \\
37.0, \text{ t} \\
31.8, \text{ t} \\
25.0, \text{ t} \\
22.6, \text{ t} \\
14.0, \text{ q}
\end{align*} \]

There is only one branch point, where the OH is attached. Therefore the rest of the molecule is linear.

\[ \begin{align*}
14.1 & \quad 32.2 & \quad 23.1 \\
23.1 & \quad 32.2 & \quad 14.1
\end{align*} \]

The chemical shifts of hexane are the replicated in the data, suggesting that the alcohol is at one end of the chain, not shifting the other end.

Calculated chemical shifts

\[ \begin{align*}
14.1 & \quad 32.2 & \quad 39.1 \\
23.1 & \quad 29.7 & \quad 82.1
\end{align*} \]

With two groups alpha on the carbon, the calculated chemical shift is too high.
3. (40 points)  \( \text{C}_5\text{H}_9\text{N} \)  \( \text{IHD} = 2 \)

**There is one H not on C, therefore on the N**

127.1, d  
125.6, d  
45.0, t  
43.1, t  
25.9, t

\[ 127.1 \quad 125.6 \]  
The alkene is not symmetrical

\[ \Theta \]  
There is one ring with no branch points, so all the C's and the N have to be contained in the ring

Using generic chemical shifts, we calculate the \( \text{RCH}_2\text{NH} \) would come at about 51. We have 45.0, t and 43.1, t

Putting it all together

Why would \( \text{not fit the data?} \)