Last Name	First Name	MI
Student ID Number:		Total Score
Circle the name of your TA: MIKE ROB		
Discussion Section – Day: Time:		/ 100

Chem 30B Spring 2004

MIDTERM #2

(50 Min)

Weds May 26th

INTERPRETATION OF THE QUESTIONS IS PART OF THE EXAM – DO NOT ASK FOR THE QUESTIONS TO BE EXPLAINED TO YOU

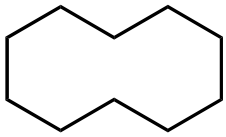
ONLY ANSWERS WRITTEN IN THE BOXES PROVIDED WILL BE GRADED

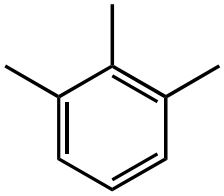
****DO NOT OPEN THIS EXAM UNTIL INSTRUCTED TO DO SO****

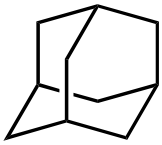
Q1	/ 20	Q4	/ 15
Q2	/ 20	Q5	/ 30
Q3	/ 15	Bonus	/ 15
		Total	/ 100

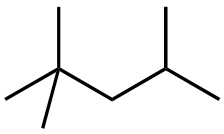
"Marge, don't discourage the boy! Weaseling out of things is important to learn. It's what separates us from the animals ... except the weasel." – Homer Simpson

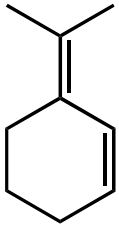
1. Predict the number of signals you would expect to see in the 1H-decoupled 13C-NMR spectrum of each of the molecules shown below. (2 points each)

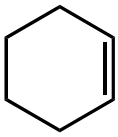
(a)  ☐

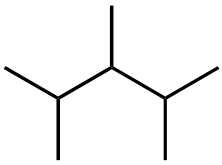
(b)  ☐

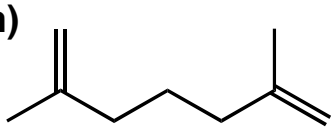
(c)  ☐

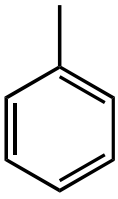
(d)  ☐

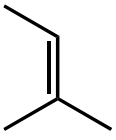
(e)  ☐

(f)  ☐

(g)  ☐

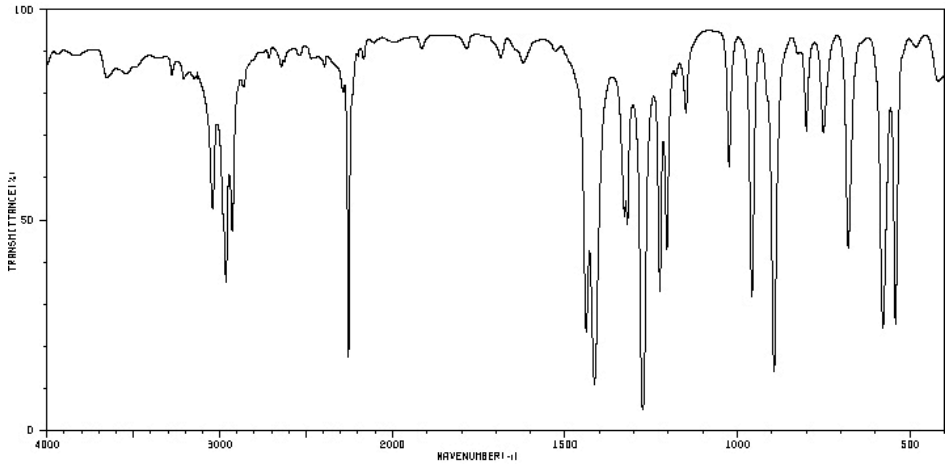
(h)  ☐

(i)  ☐

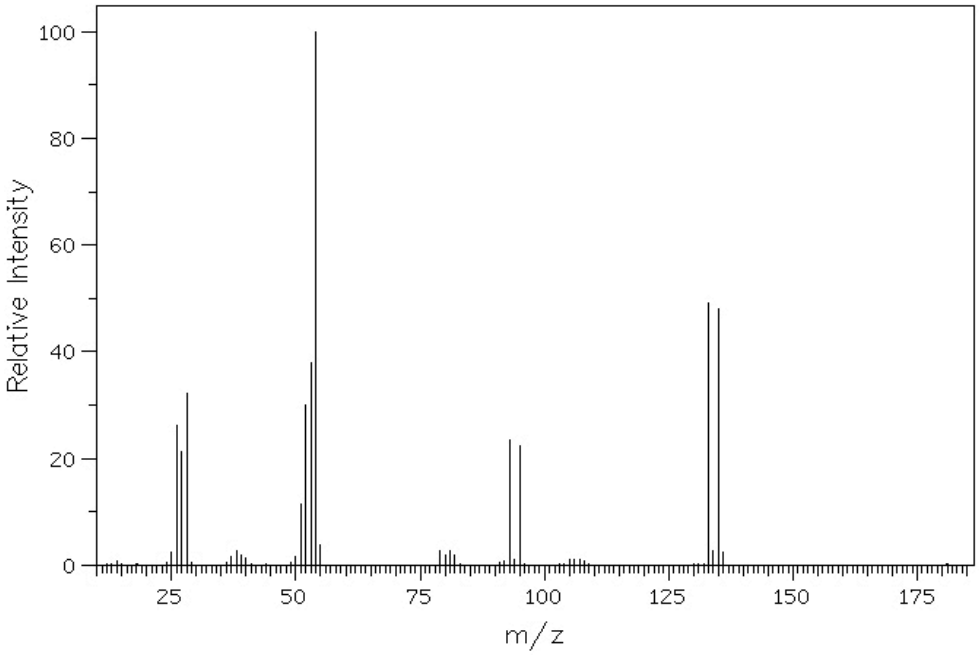
(j)  ☐

2. Some spectroscopic data for an unknown compound (**A**) are shown below. Use these data to answer the questions on the following page.

IR Spectrum



Mass Spectrum



The base peak (100% intensity) is at m/z = 54. The peaks at m/z = 133, 134, 135, and 136, have the following relative intensities (49:2:48:2), respectively.

1H-NMR Spectrum

δ = 3.0 (triplet, integration = 1), δ = 3.5 (triplet, integration = 1) ppm

13C-NMR Spectrum

δ = 22, 25, 117 ppm

(a) What is the molecular formula of compound **A**? (3 points)

(b) What is the structure of compound **A**? (10 points)

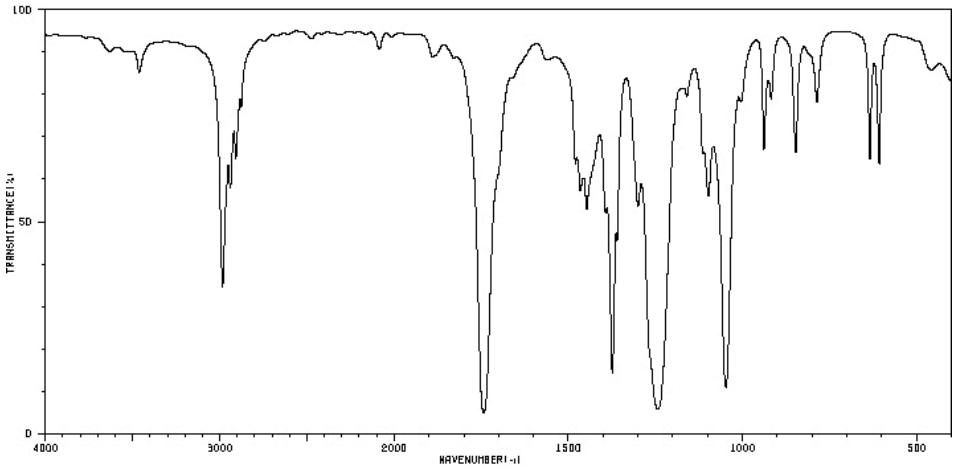
(c) What is the **precise** structure of the fragment that gives rise to a peak at $m/z = 93$? (2 points)

(d) What is the **precise** structure of the fragment that gives rise to a peak at $m/z = 95$? (Your answer should differ from that given in part (c)) (2 points)

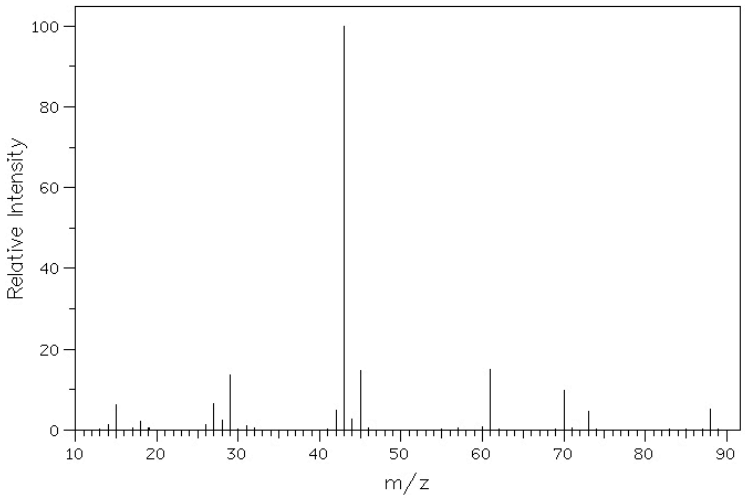
(e) What is the structure of the fragment that gives rise to the base peak at $m/z = 54$? (3 points)

3. Some spectroscopic data for an unknown compound (**B**) are shown below. Use these data to answer the questions on the following page.

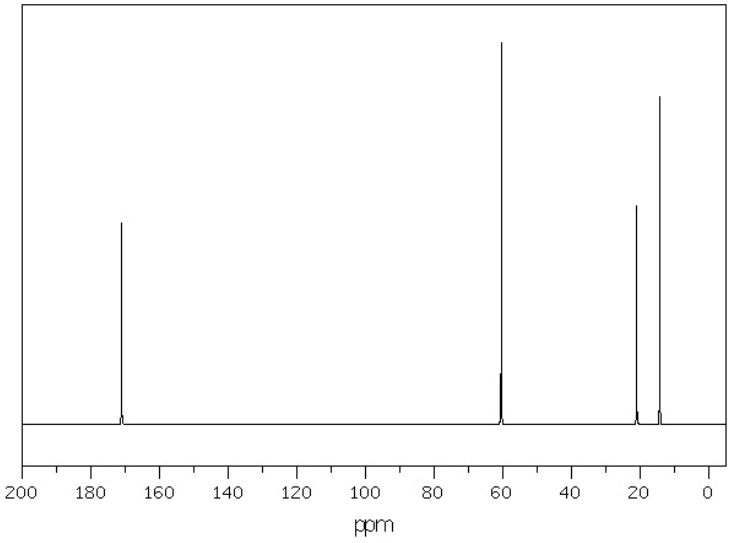
IR Spectrum



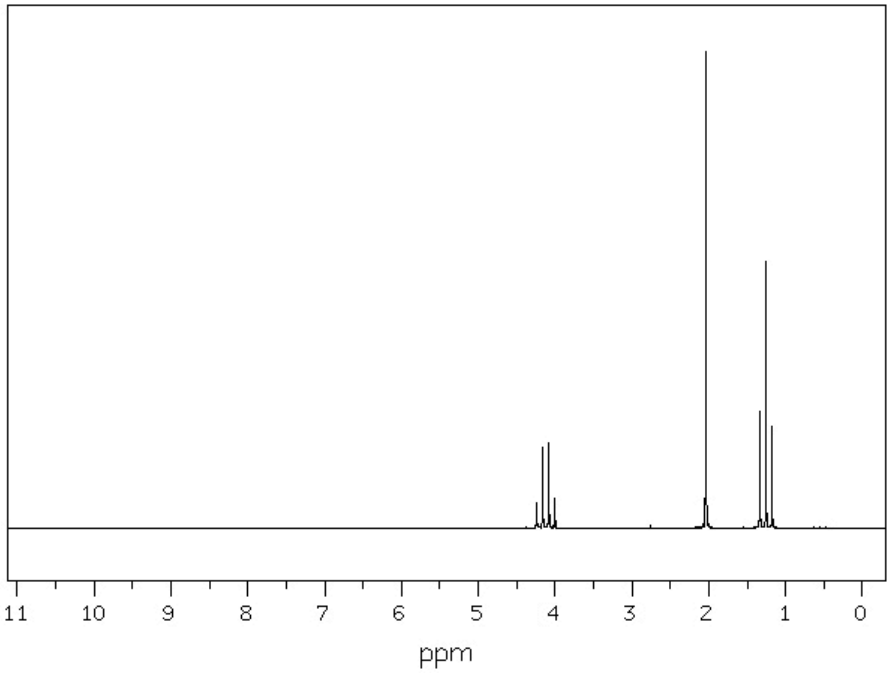
Mass Spectrum



13C-NMR Spectrum



1H-NMR Spectrum



The relative integration of the peak groupings from left to right are 2:3:3

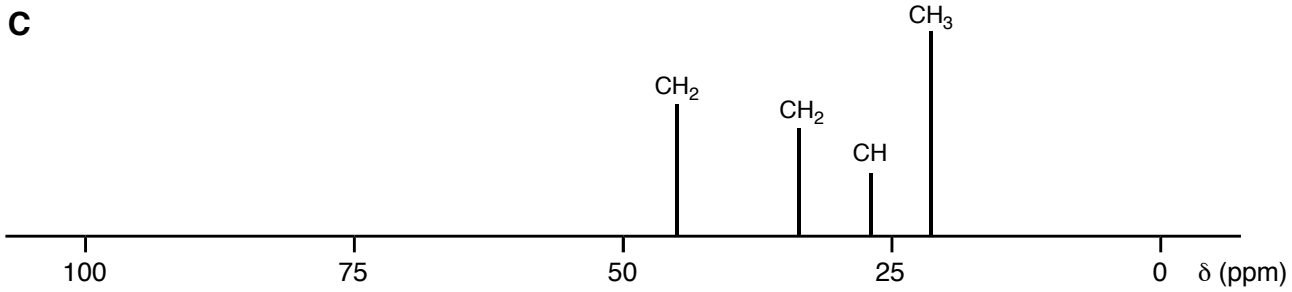
(a) What is the molecular formula of compound **B**? (3 points)

(b) What is the structure of compound **B**? (10 points)

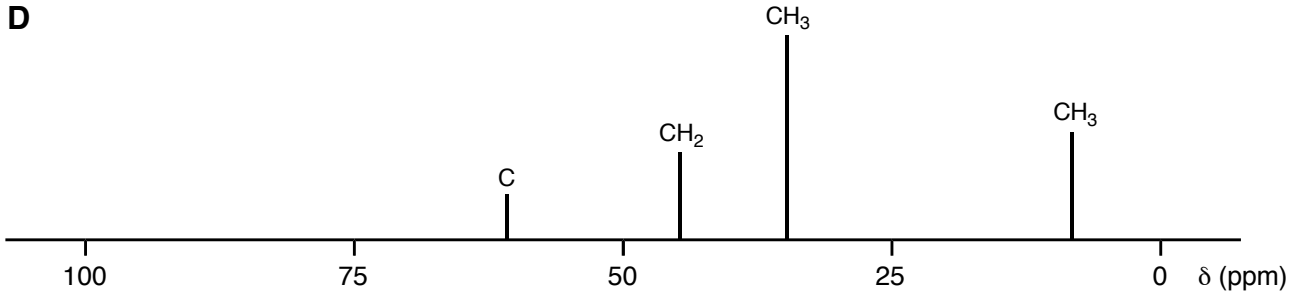
(c) What is the structure of the fragment that gives rise to the base peak at $m/z = 43$? (2 points)

4. Compounds **C**, **D**, and **E** are isomers with the molecular formula $C_5H_{11}Br$. The 1H-decoupled 13C-NMR spectrum of each compound is shown below, with the assignment from the DEPT spectrum shown above each peak (All peaks are shown, there are no peaks at ppm values > 100). In the boxes provided below, draw the structures of **C**, **D**, and **E**, based upon these spectra. (5 points each)

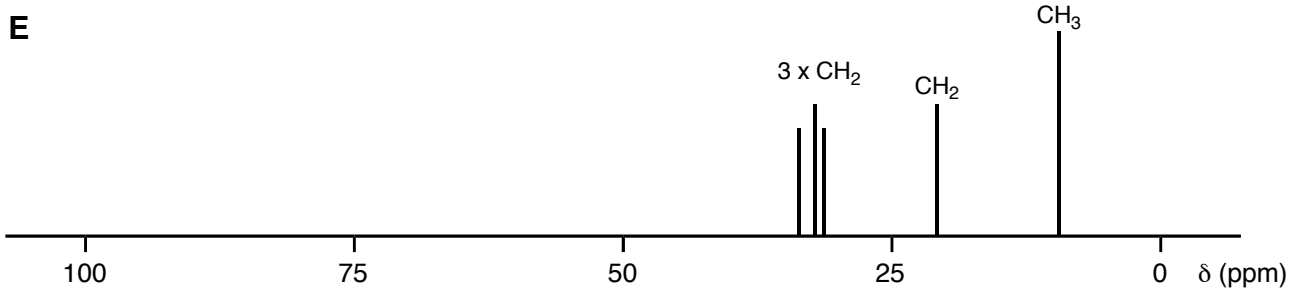
C



D



E



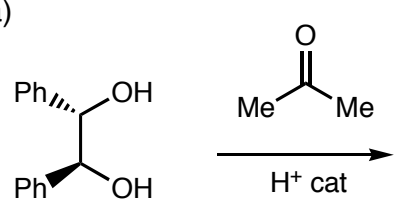
C

D

E

5. The diols shown below react with ketones (acetone in a and b; methyl ethyl ketone in c and d) to form cyclic ketals. In each case, draw the product of the reaction (**F**, **G**, and **H**), note: in d, two different diastereomeric products (**J** and **K**) are formed. In parts a and b, predict how many methyl signals will be observed in the 1H NMR spectra of compounds **F** and **G**, respectively. In compounds **H**, **J**, and **K**, what are the stereotopical relationships between the phenyl groups in each case. (3 points per box)

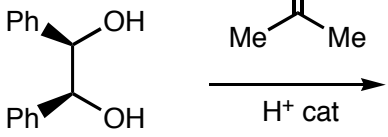
(a)



F

Number of methyl signals in 1H NMR spectrum of **F**?

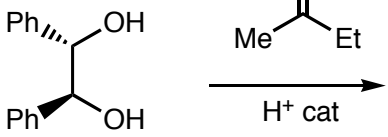
(b)



G

Number of methyl signals in 1H NMR spectrum of **G**?

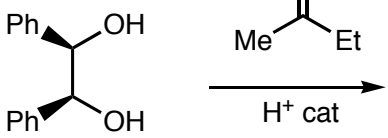
(c)



H

Topicity of Ph groups (Homotopic / Enantiotopic / Diastereotopic) in **H**?

(d)



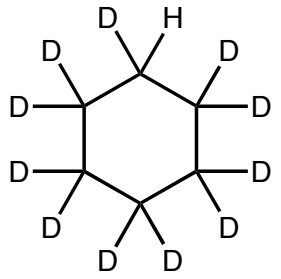
J + **K**

Topicity of Ph groups (Homotopic / Enantiotopic / Diastereotopic) in **J**?

Topicity of Ph groups (Homotopic / Enantiotopic / Diastereotopic) in **K**?

6 (BONUS) At –100 °C, undecadeuteriocyclohexane (**L**) gives rise to two equal intensity signals in the 1H-NMR spectrum. In contrast, at room temperature, only one signal is observed in the 1H-NMR spectrum.

L



(a) Draw the two different species (**L1** and **L2**) that give rise to the signals at –100 °C (3 points each)

L1

L2

(b) Briefly explain why only one signal is observed in the 1H-NMR spectrum when it is recorded at room temperature (4 points)

7 (BONUS) Compound **M** has the molecular formula $C_4H_8O_2$. Only one peak is observed in the 1H-decoupled 13C-NMR spectrum, and only one singlet is observed in the 1H-NMR spectrum. Propose a structure for **M**. (5 points)

M

Otherwise Blank Page