

Seat No. _____

LAST NAME WST

Section _____

FIRST NAME _____

**PLEASE REMOVE LAST PAGE OF EXAM BEFORE PRINTING YOUR NAME
ON THE BACK OF PAGE 8.
THERE ARE 9 PAGES TO THIS EXAM. CHECK TO MAKE SURE
YOU HAVE A COMPLETE EXAM.**

CHEMISTRY 331

EXAM V

Spring 2007
April 20, 2007

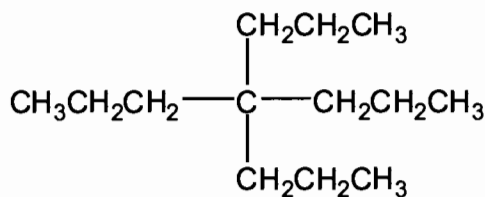
- I. (16 points) _____
- II. (13 points) _____
- III. (8 points) _____
- IV. A, B & C (21 points) _____
- D, E & F (21 points) _____
- V. (21 points) _____
- TOTAL (100 points) _____

The Final Exam is scheduled for Monday, April 30, from 7:30-9:30 A.M.

First 4 exams scores (to be filled in by graders). Best 4 (including score above) will be counted in your final score.

_____	_____	_____	_____	_____
I	II	III	IV	# of quizzes taken (Maximum score = 10)

- I. (16 pts.) A. (8 pts.) The mass spectrum of hydrocarbon A (molecular formula is $C_{13}H_{28}$) shows a parent peak and a strong fragmentation peak at lower m/z values. (See the last page for a Periodic Table of the Elements.)



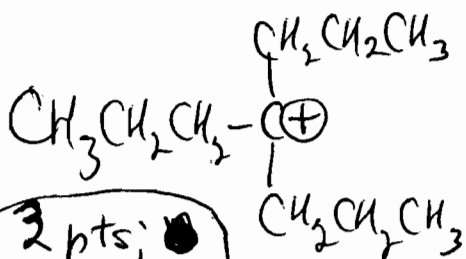
Math error
-1 pt

A

1. (3 pts.) What is the m/z value for the parent peak? 184

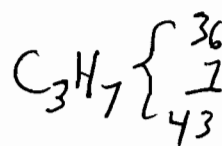
$$\begin{array}{r} 13 \\ 12 \\ \hline 26 \\ 13 \\ \hline 156 \end{array} \quad \begin{array}{r} 156 \\ 28 \\ \hline 184 \end{array}$$

2. (5 pts.) Give the expected structure and the m/z value for the major positively charged fragment.



3 pts; ●
1 pt if not +

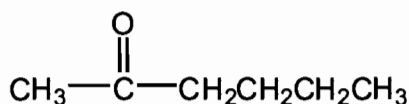
$$\begin{array}{r} 12 \\ 10 \\ \hline 120 \\ +21 \\ \hline 141 \end{array} \quad \text{or} \quad \begin{array}{r} 184 \\ 43 \\ \hline 141 \end{array}$$



141

2 pt

- B. (8 pts.) The mass spectrum of ketone B (molecular formula is $C_6H_{12}O$) shows a parent peak and two very strong fragmentation peaks at lower m/z values.

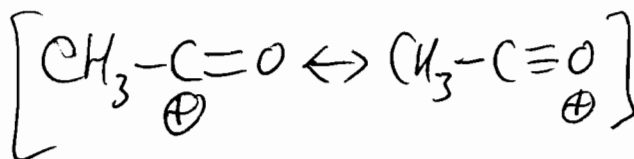


B

3. (3 pts.) What is the m/z value for the parent peak? 100

$$\begin{array}{r} 12 \\ 6 \\ \hline 72 \end{array} \quad \begin{array}{r} 72 \\ 12 \\ \hline 16 \\ 100 \end{array}$$

4. (5 pts.) Give the expected structure and the m/z value for the lower molecular weight positively charged fragment.



3 pts for either structure

24

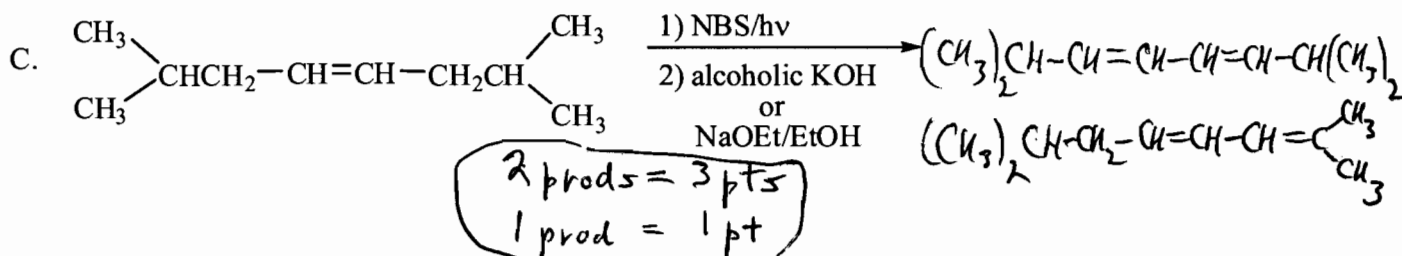
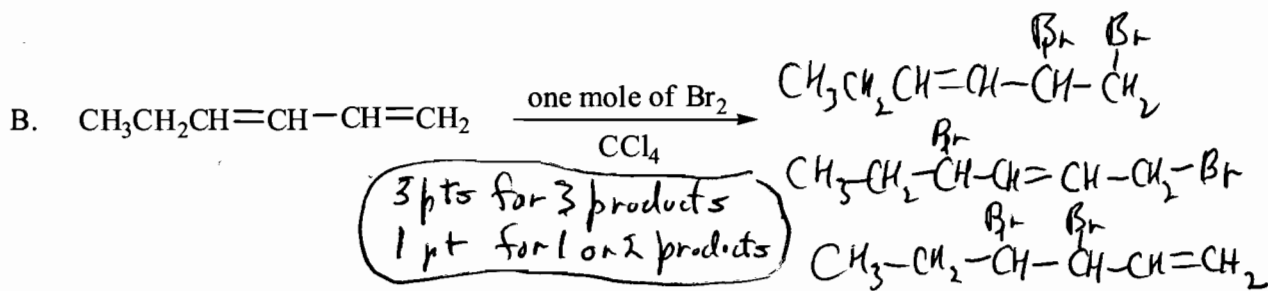
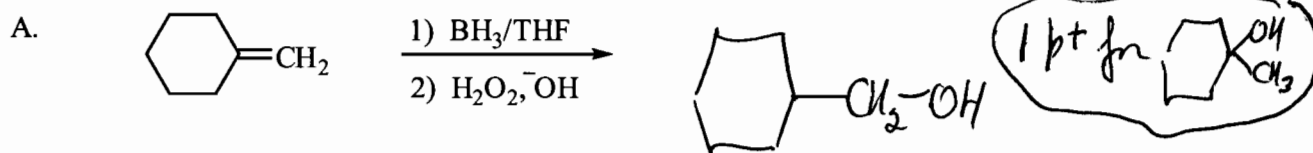
3

16

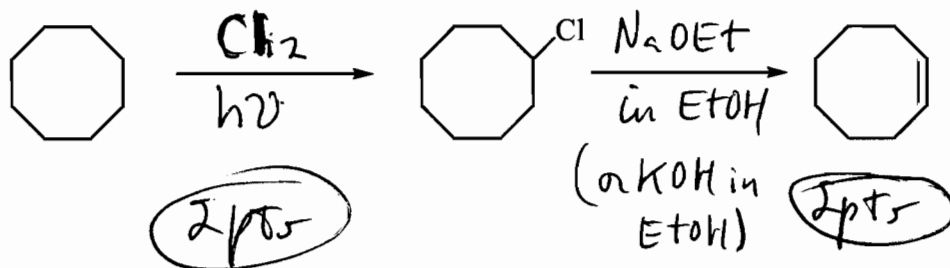
43

2 pts

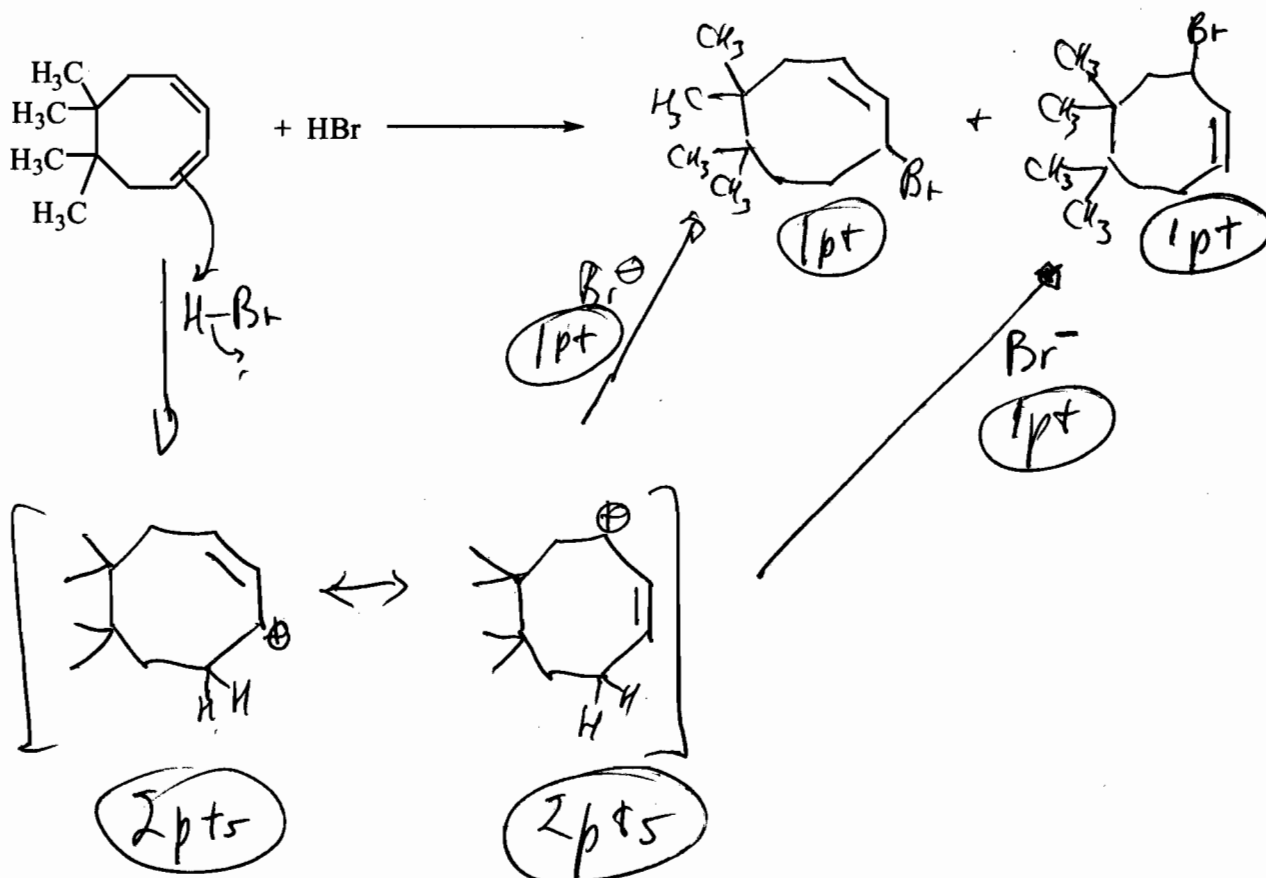
- II. (13 pts) Complete the following equations, giving all organic product(s). No stereochemistry required.



- D. (4 pts) Give the reactants for the following reactions.



III. (8 pts) Give the product(s) (neglect stereochemistry) and draw a stepwise mechanism for the following reaction (include all important resonance structures).



-1pt for showing a duplicate structure

-1pt for each incorrect product

4/2/08

IV. (42 pts) For each of the following compounds, propose a structure in the box provided that fits the data presented.

A. (7 pts)



^1H NMR:

δ 3.9 (2H, singlet)

δ 2.7 (2H, quartet)

δ 1.1 (3H, triplet)

Broadband-decoupled ^{13}C NMR:

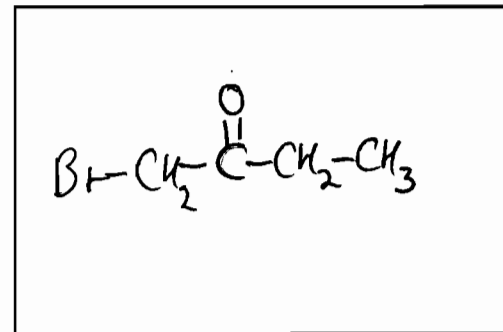
δ 202.60

δ 34.09

δ 33.16

δ 7.93

IR: 1710cm^{-1}



2 pts for $-\text{C}-$

-2 pts for minor error (e.g., Cl instead of Br)

B. (7 pts)



^1H NMR:

δ 2.3 (2H, singlet)

δ 2.1 (3H, singlet)

δ 1.0 (9H, singlet)

Broadband-decoupled ^{13}C NMR:

δ 208.38

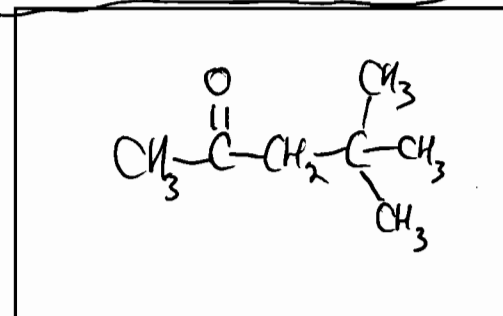
δ 56.00

δ 32.30

δ 30.91

δ 29.77

IR: 1710cm^{-1}



2 pts for $-\text{C}-$

C. (7 pts)



^1H NMR:

δ 2.4 (2H, triplet)

δ 2.1 (3H, singlet)

δ 1.6 (2H, multiplet)

δ 1.3 (6H, multiplet)

δ 0.9 (3H, triplet)

Broadband-decoupled ^{13}C NMR:

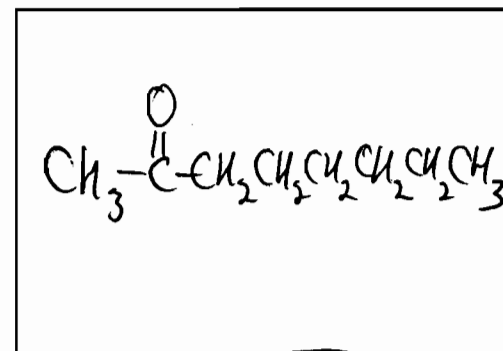
δ 209.58 δ 29.77

δ 44.67 δ 24.80

δ 32.48 δ 23.35

δ 30.54 δ 14.80

IR: 1710cm^{-1}



2 pts for $-\text{C}-$

D. (7 pts) $C_7H_4Cl_4O$

1H NMR:

δ 7.4 (1H, singlet)

δ 3.9 (3H, singlet)

Broadband-decoupled ^{13}C NMR:

δ 154.54

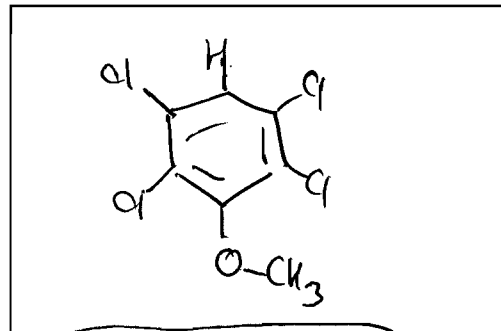
δ 131.94

δ 127.38

δ 126.33

δ 60.75

IR: 1100 cm^{-1}



phenyl ring + 2 pts

E. (7 pts) C_8H_{14}

1H NMR:

δ 5.8 (2H, multiplet)

δ 5.0 (4H, multiplet)

δ 2.1 (4H, multiplet)

δ 1.4 (4H, multiplet)

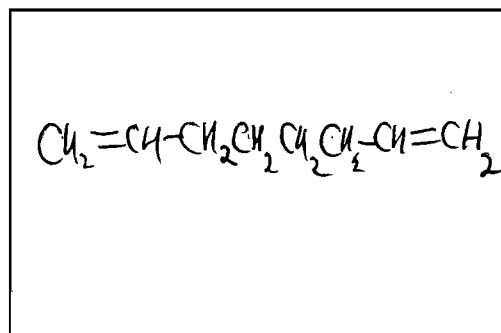
Broadband-decoupled ^{13}C NMR:

δ 138.89

δ 114.25

δ 33.65

δ 28.43



F. (7 pts) The following compound is characterized by a 1H NMR spectrum that consists of only a single peak (a singlet) having the chemical shift indicated. Some additional data are given. Write the correct structure for the compound (either of two structures will get full credit) in the appropriate box.

$C_8H_{12}O_2$

1H NMR:

δ 1.3 (12H, singlet)

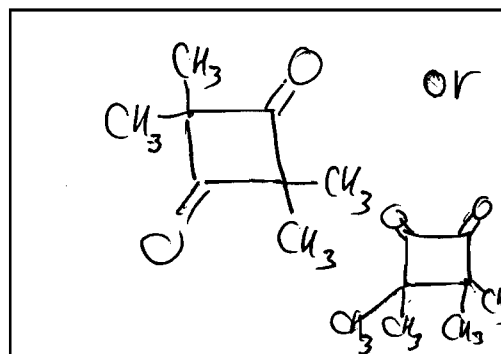
Broadband-decoupled ^{13}C NMR:

δ 215.42

δ 70.37

δ 18.82

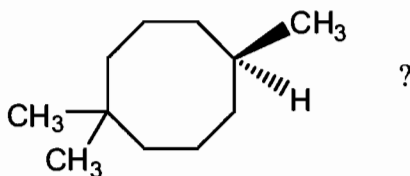
IR: 1750 cm^{-1}



or + 2 pts

V. (21 pts) Circle the correct answer (think carefully).

A. How many signals are present in the broadband-decoupled ^{13}C NMR spectrum of



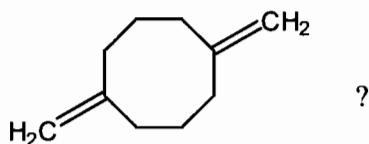
1.) 7

2.) 8

3.) 10

4.) 11

B. How many signals are present in the ^1H NMR spectrum of



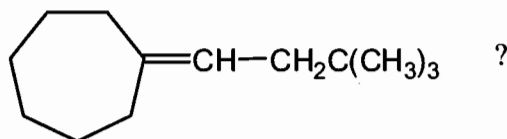
1.) 3

2.) 4

3.) 5

4.) 6

C. How many signals are present in the broadband-decoupled ^{13}C NMR spectrum of



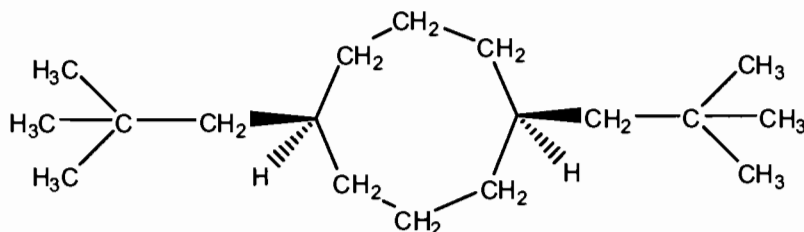
1.) 8

2.) 9

3.) 11

4.) 12

D. The DEPT 90 ^{13}C NMR spectrum of



would show how many signals?

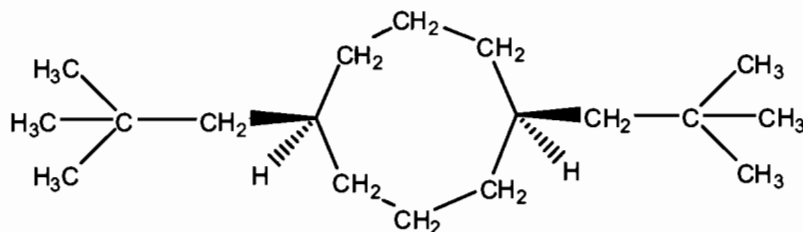
1.) 1

2.) 2

3.) 4

4.) 5

E. The DEPT 135 ^{13}C NMR spectrum of



would show how many positive and how many negative signals?

1.) 2 positive, 2 negative

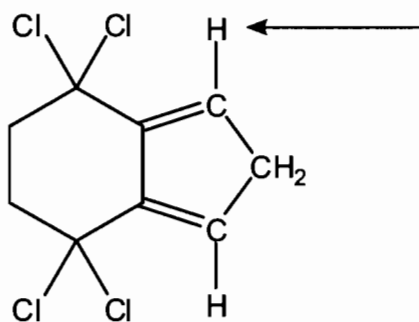
2.) 2 positive, 3 negative

3.) 4 positive, 3 negative

4.) 4 positive, 5 negative

Not correct.

F. What multiplicity (splitting pattern) is observed in the ^1H NMR spectrum for the indicated hydrogen?



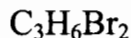
1.) Singlet

2.) Doublet

3.) Triplet

4.) Quartet

G. The natural abundance of bromine isotopes is 50.7% ^{79}Br and 49.3% ^{81}Br . The molecular ion region of the mass spectrum of compound G would be expected to show



G

1. One peak at $m/z = 202$

2. Two peaks at $m/z = 200$ and $m/z = 202$

3. Two peaks at $m/z = 200$ and $m/z = 204$

4. Three peaks at $m/z = 200$, $m/z = 202$, and $m/z = 204$

$$\begin{array}{r} 12 \\ \times 3 \\ \hline \end{array}$$

$$36$$

$$6$$

$$79$$

$$79$$

$$200$$