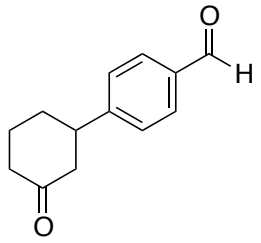
Chem 333

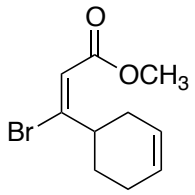
Name____Key_____

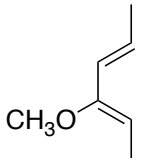
Fall 2012
Exam #3
November 19, 2012

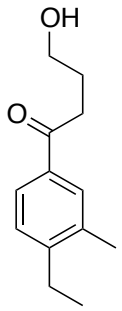
This is an open-notes, open-book exam. For #1, indicate which UV table should be used, and calculate the $\lambda_{max}$. For #2, calculate the percent of **A** that has been converted to **B**. For #3 and for #4, deduce the structure of the product.

1. (20 points)

1. 

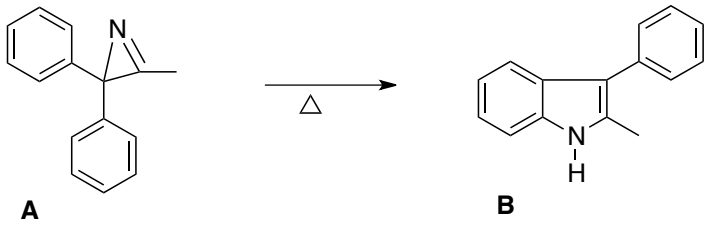

2. 


3. 


4. 

2. (10 points)

On heating, **A** is converted into **B**. A sample of **B** showed an absorbance at 220 nm of 2.30, and an absorbance at 280 nm of 1.80 nm. A sample of **A** showed an absorbance at 220 nm of 1.85, and an absorbance at 280 nm of 0.65. After an hour at 165° C, a sample that at the beginning had been pure **A** showed an absorbance at 220 nm of 1.70, and an absorbance at 280 nm of 1.00. What percent of **A** had been converted to **B**?




**A** **B**

Proportional reasoning. A sample of pure **A** that showed an absorbance at 220 nm of 1.70 would show an absorbance at 280 nm of .597. A sample of pure **B** that showed an absorbance at 220 nm of 1.70 should show an absorbance at 280 nm of 1.33. It follows that the sample is 55% **B**.

3. (30 points) Deduce the structure of **C**.

**C** $C_{10}H_{11}NO$

**$^{1}$H NMR:**
7.6, , bs, 1H (exchanges)
6-7-7.3, m, 5H
6.02, ddt, J = 15.5, 11.2, 7.2 Hz, 1H
5.35, d, J = 15.5 Hz, 1H
5.22, d, J = 11.2 Hz, 1H
3.22, d, J = 7.2 Hz, 2H

**$^{13}$C NMR:**
169.0, s
137.4, s
131.1, d
129.0, d (2)
124.4, d
120.5, t
119.9, d (2)
42.7, t

1. IHD = 6, on H on N or O

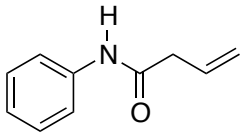
2. One carbonyl at 169.0, s, a carboxylic acid derivative

IHD of 4 = three double bonds and a ring, a benzene derivative, confirmed by 6.7-7.3, 5H. So, one substituent on the benzene ring. From 119.9, d (2), the N is directly attached to the ring

One more alkene, 120.5, t plus one d, so -CH=$CH_2$

From 6.02, ddt, there is one more CH2: -$CH_2$-CH=$CH_2$

Putting it all together:



4. (40 points) Deduce the structure of **D**.

**D** $C_{10}H_{10}O_3$ IR: 2916, 1247, 1025, 776, 600 $cm^{-1}$

**$^1$H NMR:**
2.67 dd, 1H, *J* = 8.2, 3.9 Hz
2.79 dd, 1H, *J* = 8.2,1.1 Hz
2.99 d, 2H, *J* = 6.6 Hz
3.56 m, 1H
5.87 s, 2H
6.56–6.6 m, 3H

**$^{13}$C NMR:**
14.4, t
46.7, t
51.9, d
96.1, t
114.1, d
118.3, d
124.2, d
131.9,s
147.1, s
149.2, s

1. IHD = 6, all H's on carbon

2. Benzene ring, trisubstituted. From 147.1, 149.2, two O's directly attached to the ring, one C. From 114.1, d and118.3, d, two positions ortho to the oxygens are C-H

There are two more rings

3. One of the rings is a monosubstituted epoxide 46.7, t 51.9, d. The $CH_2$ shows up at 2.67 and 2.79. The C-H is at 3.56

That leaves two more O's. From 96.1, t, there is O-$CH_2$-O. We know that two of the O's are attached to the ring

Putting it all together: