Chemistry 3331-100
Organic Chemistry/Dr. Barney Ellison
Thursday: Sept. 28 @ 7:00pm → 9:00/1st Exam/Hale 270

Name: Key (please print)

1. (15 pts) Identify the C_3H_5Br isomers on the basis of the following NMR results. Explain your reasoning.

a) Isomer A has three peaks in its ^{13}C NMR spectrum: δ 32.6 ppm, δ 118.8 ppm, and δ 134.2 ppm. $CH_2=CH-CH_2Br$ Has three diff carbons.

b) Isomer B has two peaks in its ^{13}C NMR spectrum: δ 12.0 ppm and δ 16.8 ppm. The peak at lower field is only half as intense as the one at higher field. CH_2 (cyclopropyl) $-CH-Br$ Has two different carbons

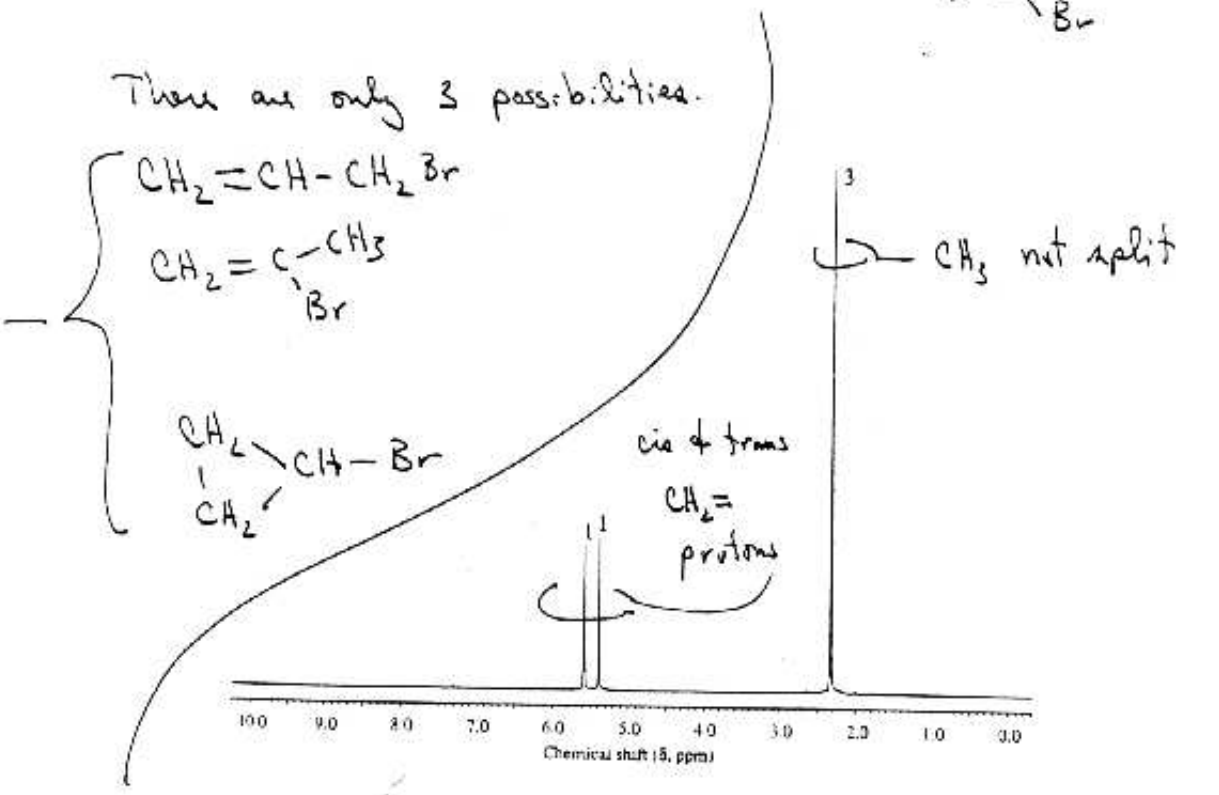
c) Isomer C has the ^1H NMR spectrum shown below. $CH_2=C(CH_3)(Br)$

There are only 3 possibilities.

$CH_2=CH-CH_2Br$

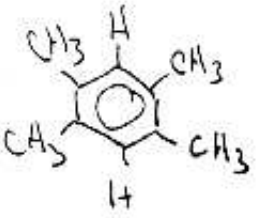
$CH_2=C(CH_3)(Br)$

CH_2 (cyclopropyl) $-CH-Br$

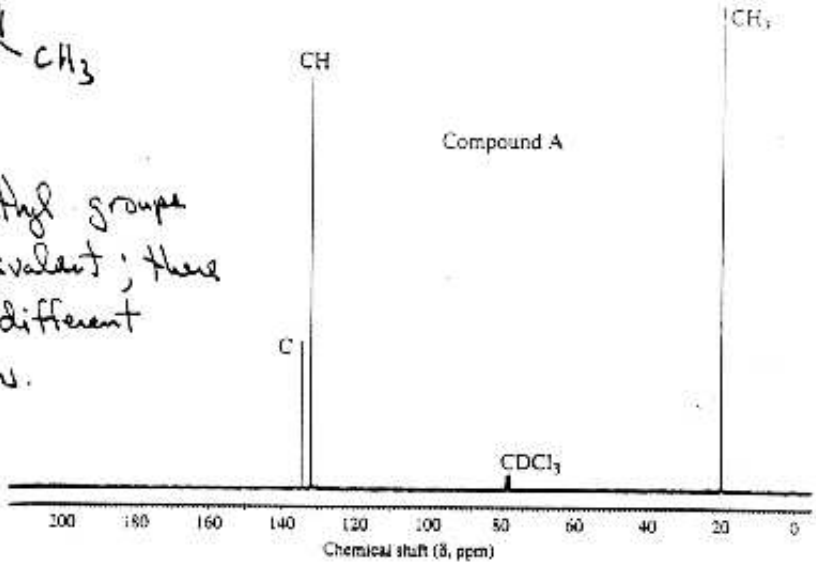


2. (10 pts) Compounds A and B are isomers with the molecular formula $C_{10}H_{12}$. Identify each one on the basis of the ^{13}C NMR spectra shown below. Explain your reasoning.

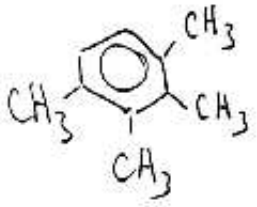
The formula tells you that an aromatic ring is present.



All methyl groups are equivalent; there are 3 different carbons.

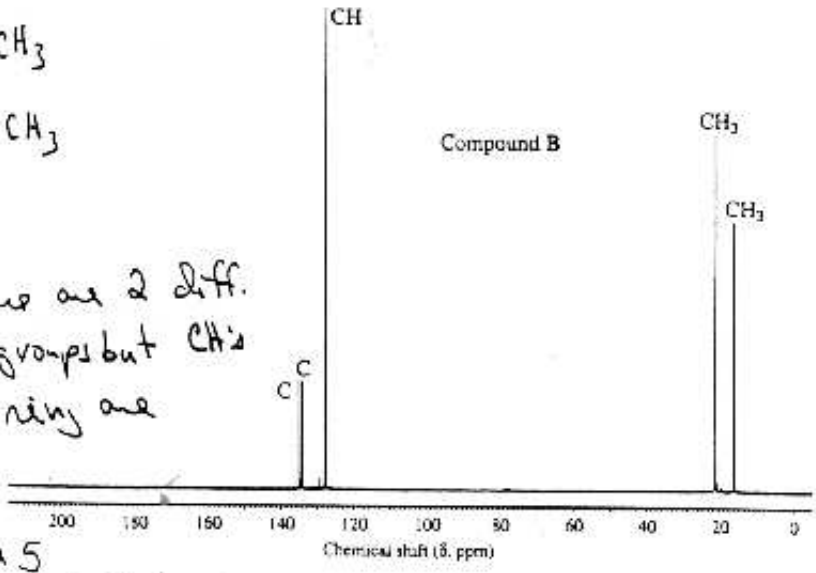


(a)

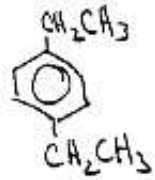


Here there are 2 diff. methyl groups but CH's on the ring are equivalent.

There are 5 different carbons.

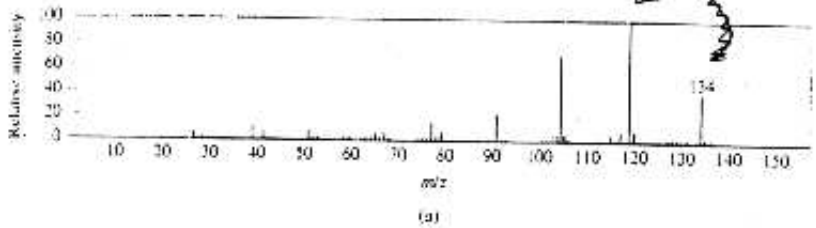


3. (10 pts) Deduce the structure of an unknown with the mass spectrum and ^{1}H NMR shown below. Explain your reasoning.



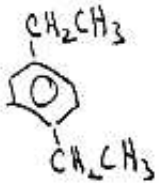
= parent peak of 134.

loss of CH_3 to produce



(a)

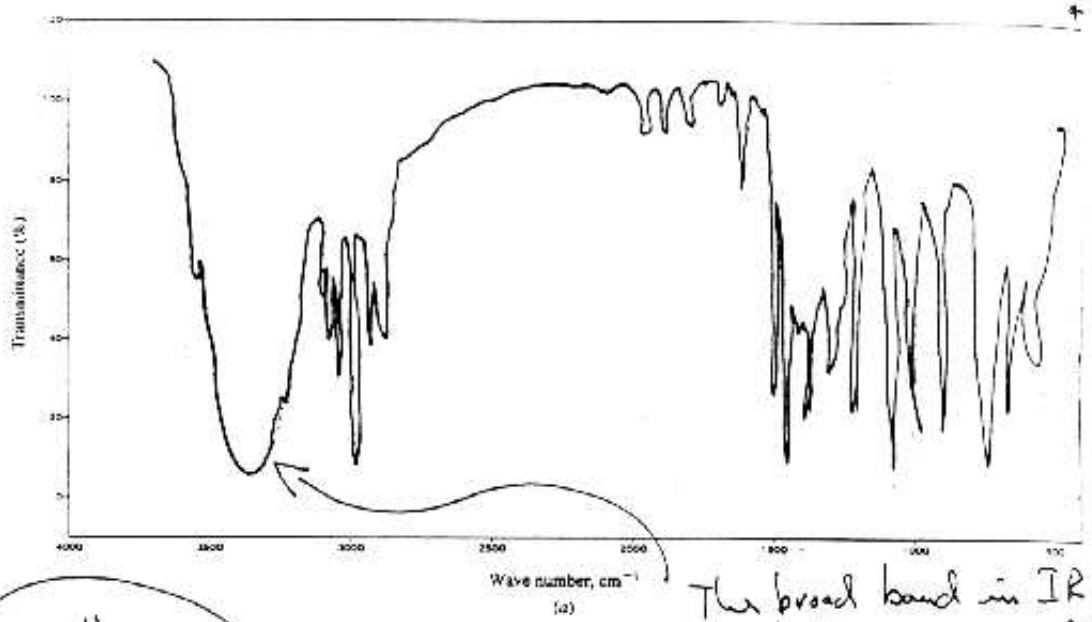
NMR can only be



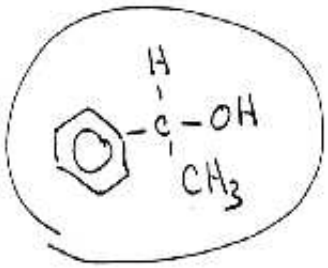
These are spin-spin splitting from the Ethyl group.

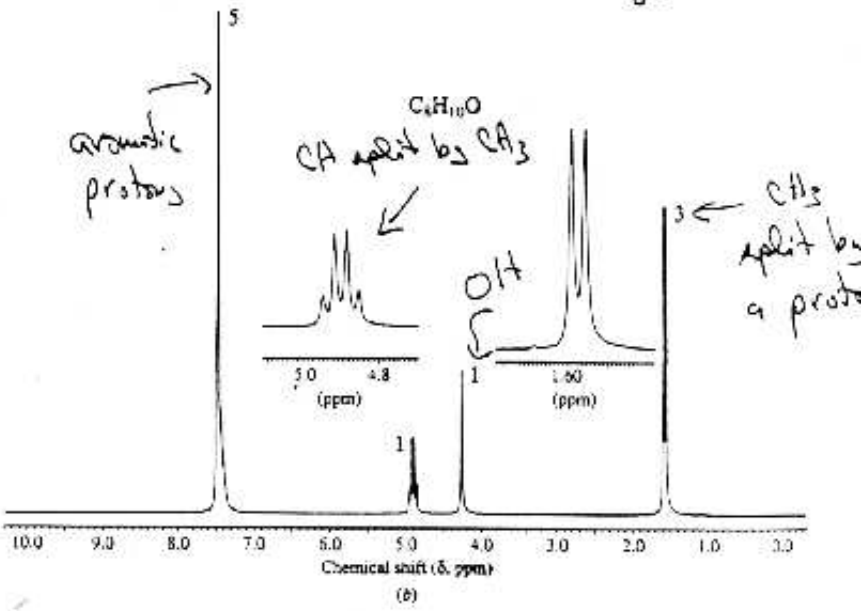
Aromatic protons

4. (10 pts) Deduce the structure of an unknown ($C_8H_{10}O$) with the infrared spectrum and ^1H NMR shown below. Explain your reasoning.



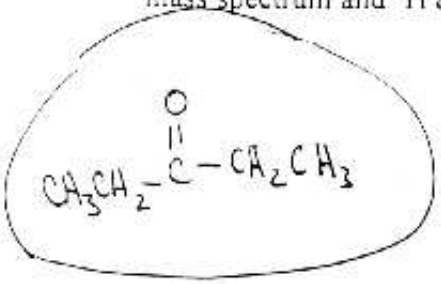
The broad band in IR tells you an alcohol





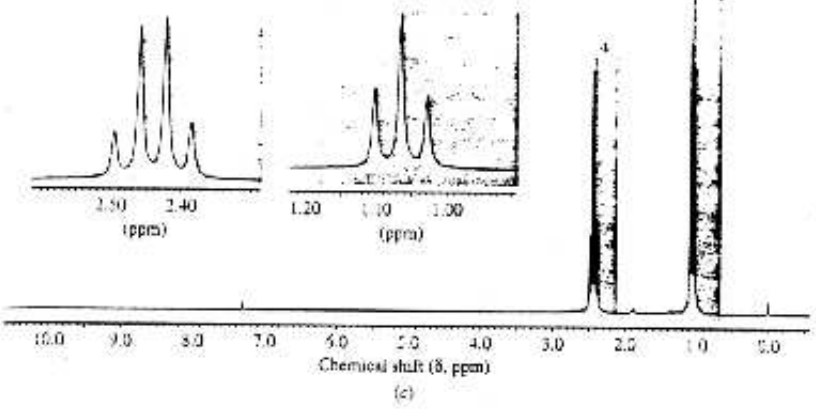
9.28.00

5. (10 pts) Deduce the structure of an unknown with the infrared spectrum, mass spectrum and ^1H & ^{13}C NMR shown below. Explain your reasoning.

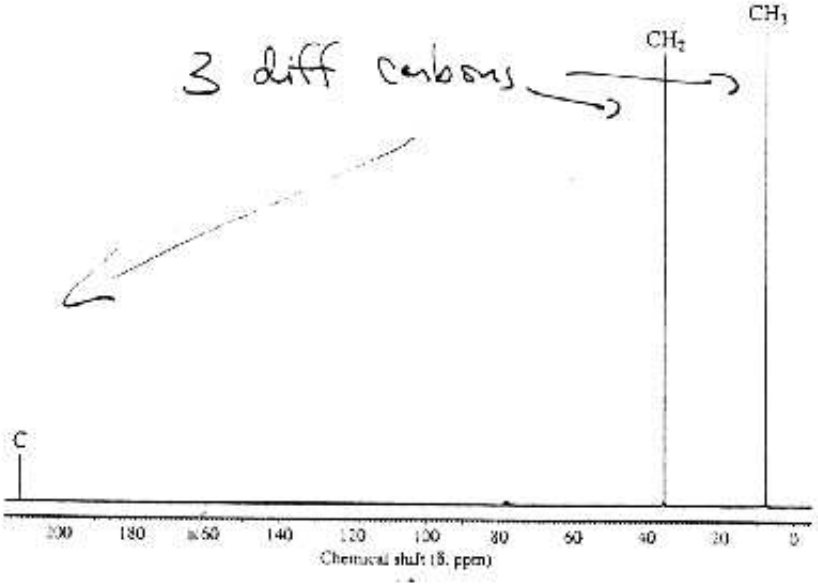


^1H NMR tells you that you only have an CH_3CH_2- grp

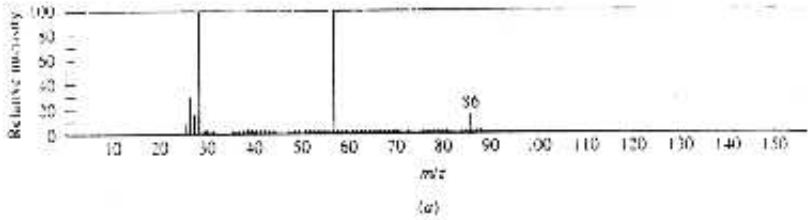
Characteristic spin-spin splitting



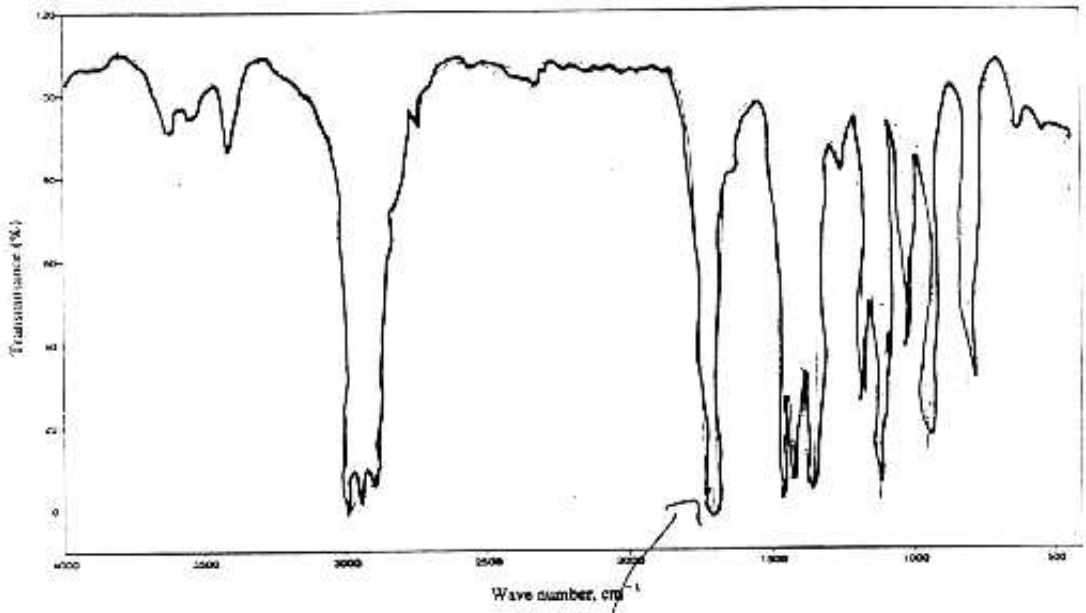
3 diff carbons



m/z 86 = parent peak



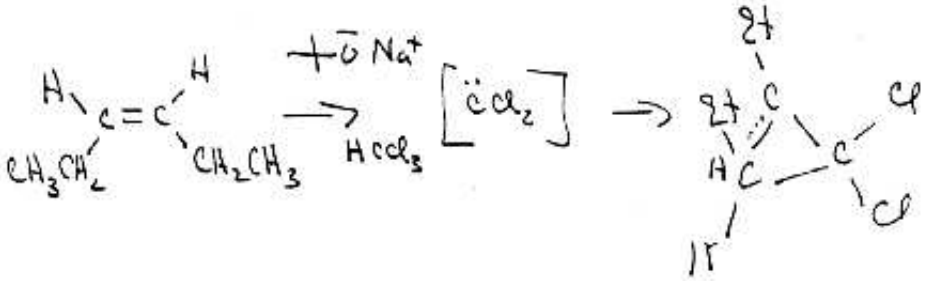
(a)



C=O stretch here

6. (15 pts) What are the products of the addition of the following reactions? Which products are achiral? Which is a racemic mixture?

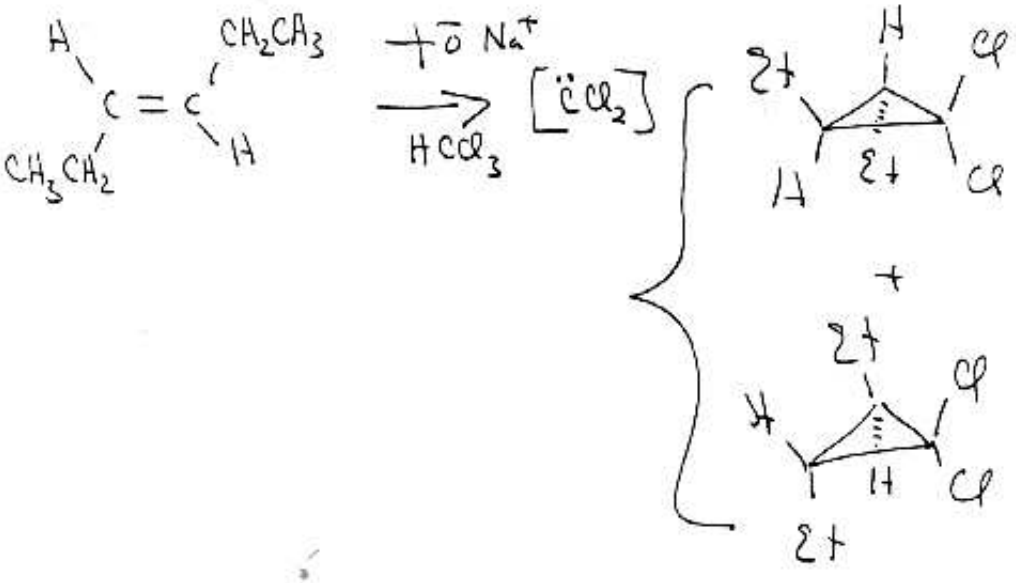
a) Z-3-hexene + $HCCl_3$ + $(CH_3)_3CO^- Na^+$ →



cis 2,3-diethyl-1,1-cyclopropane

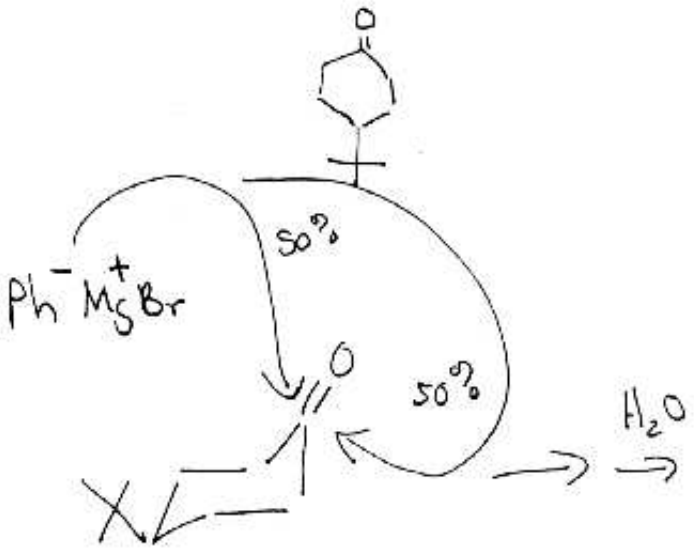
achiral

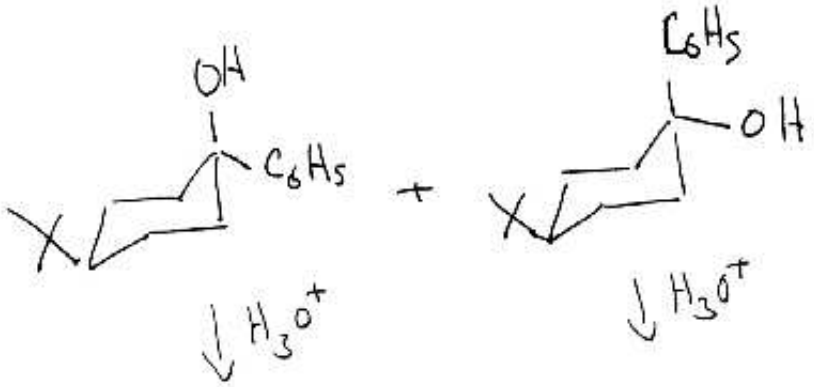
b) E-3-hexene + $HCCl_3$ + $(CH_3)_3CO^- Na^+$ →



racemic

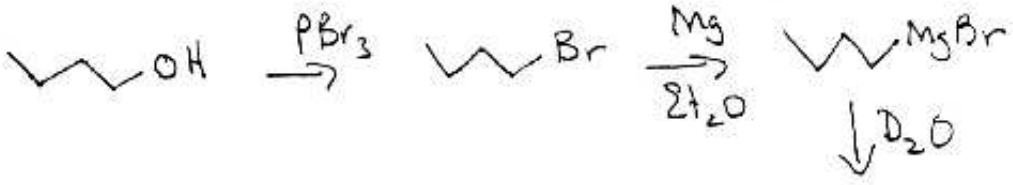
7. (10 pts) The addition of phenylmagnesium bromide to 4-*tert*-butylcyclohexanone gives two isomeric tertiary alcohols as products. Both alcohols yield the same alkene when subjected to acid-catalyzed dehydration. Suggest reasonable structures for these two alcohols.





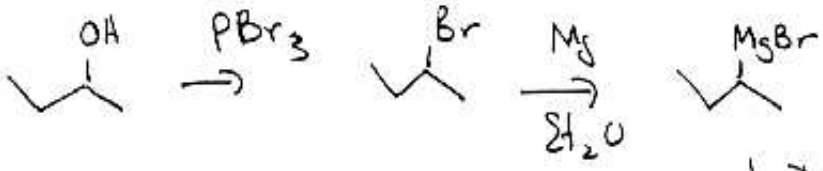
8. (10 pts) Starting with butanols of your choice and D_2O & any other inorganic reagents, prepare the following.

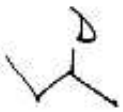
a) $CH_3CH_2CH_2CH_2D$



$CH_3CH_2CH_2CH_2D$ which is

a) $CH_3CH_2CHDCH_3$



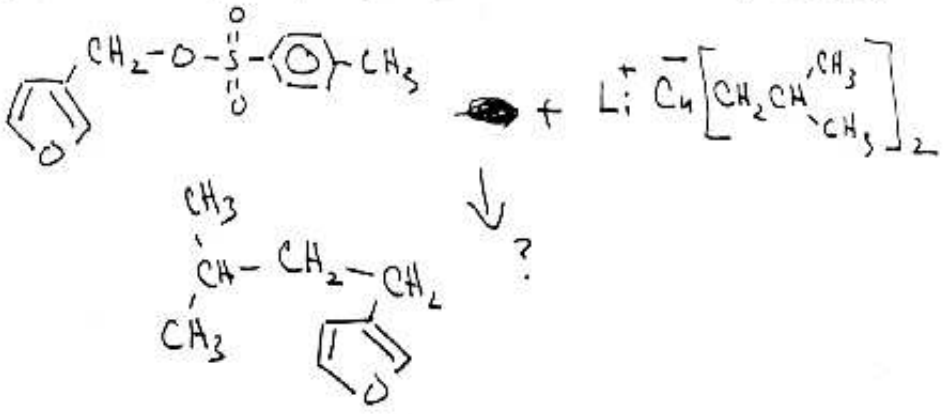


which is

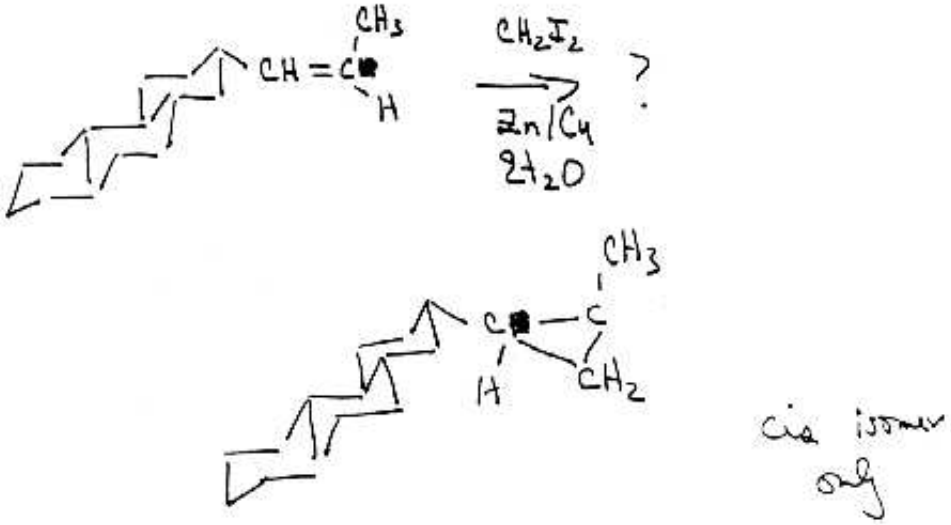
$CH_3CH_2\underset{\displaystyle D}{\underset{|}{C}}H-CH_3$

9. (20 pts) What is the principal organic product of the following reactions?

a)

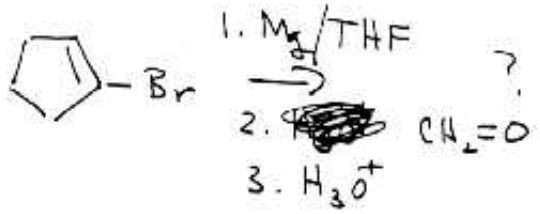


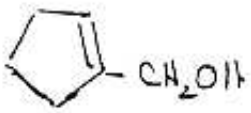
b)



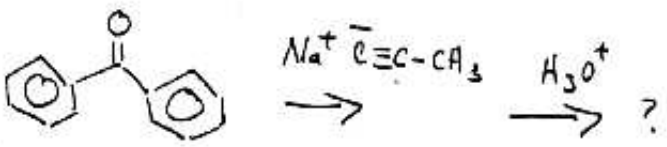
cis isomer only

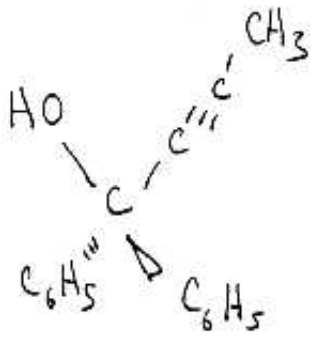
c)


1. Mg/THF
2.
3. H_3O^+
$CH_2=O$
?
Br


CH_2OH

d)


$Na^+ \bar{C}\equiv C-CH_3$
H_3O^+
?


HO
C
CH_3
C_6H_5
C_6H_5