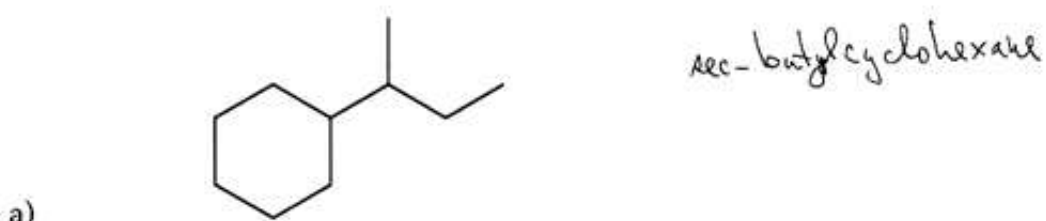


name:

Chemistry 3311-100  
Organic Chemistry / Dr. Barney Ellison  
Thursday: Feb. 10<sup>th</sup> @ 7:00pm → 9:00 / 1<sup>st</sup> Exam / Math 100

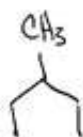
Name: Key (please print)

1. (12 pts) Write a correct name for each of the following compounds.

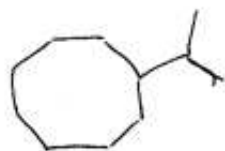


2. (8 pts) Draw a structure correctly representing the following:

a) 3-methylpentane

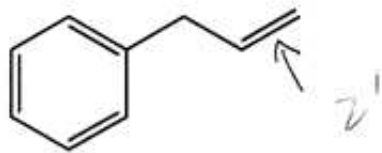


b) isopropylcyclooctane



3. (10 pts) In each of the following, choose the bond which fits.

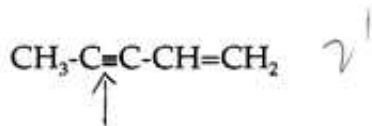
a) shortest C—C bond in:



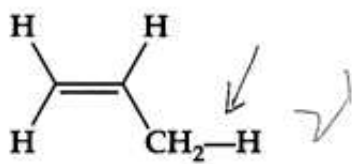
a) longest C—C bond in:



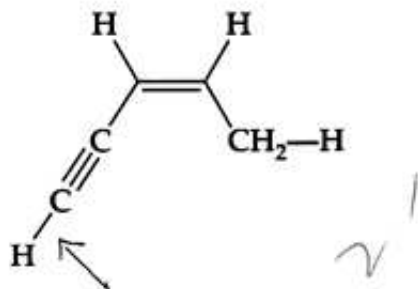
a) shortest C—C bond in:



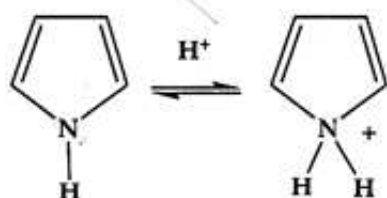
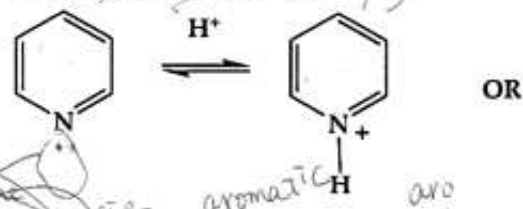
a) longest C—H bond in:



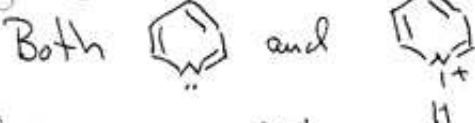
a) shortest C—H bond in:



4. (10 pts) Both pyridine and pyrrole have a lone pair of electrons on nitrogen, which can be protonated in an acid-base reaction. Remembering Hückel's rule, which protonation will be easier? Explain your reasoning.



Say one is aromatic right give



have 6- $\pi$  electrons and are aromatic.

two right give

While pyrrole is aromatic since it has 6  $\pi$  electrons.

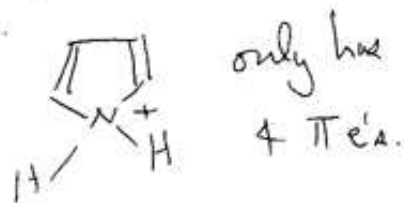


Say one right + give  
if say two right, give  
Cation is not aromatic.

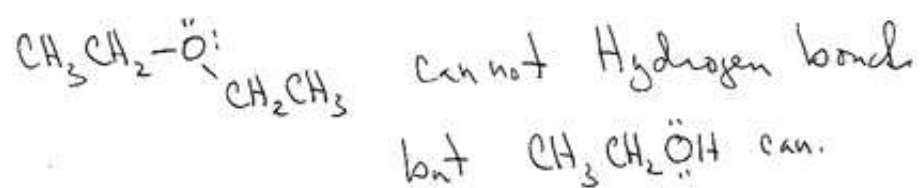
Pyridine easily protonates since both and are aromatic. 2'

But if pyrrole is protonated, aromaticity is lost & that costs a lot of energy.

is hard to protonate 2'

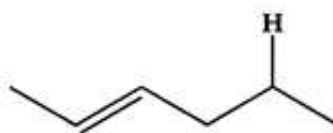
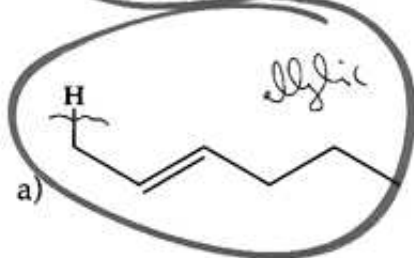
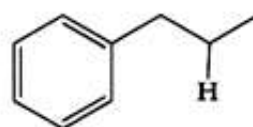
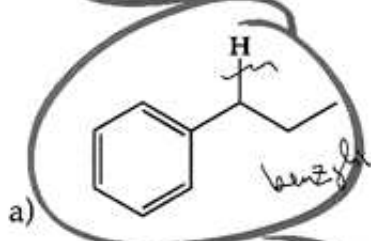
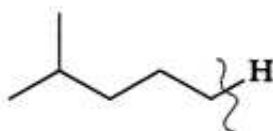
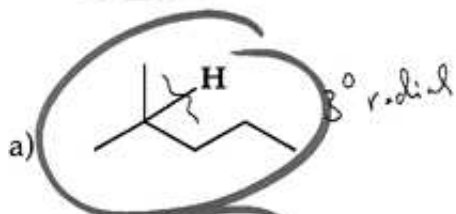
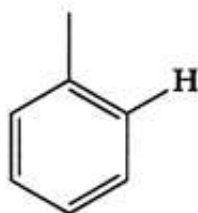
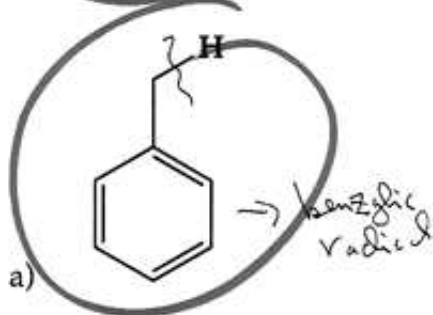
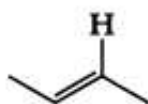
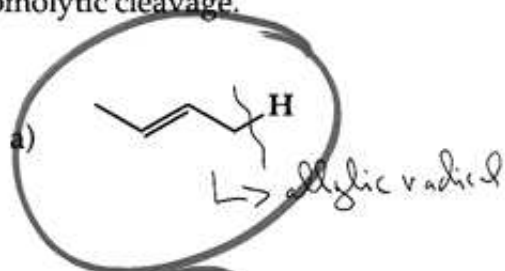


5. (10 pts) Although ethyl ether has a substantially higher molecular weight than ethanol, ethanol has a higher boiling point. Explain.



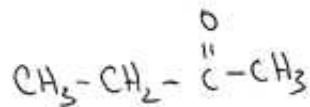
H-bonds in EtOH provide an additional  $5 \text{ kcal mol}^{-1}$  attractive force between ethanol molecules. The boiling point is raised because these additional attractive forces.

6. (10 pts) Predict which of the two indicated C—H bonds in each of the following compounds would yield a more stable radical upon homolytic cleavage.



7. (10 pts) For each of the following compounds, how many peaks would you expect to find in the  $^1\text{H}$  spectrum? What would expect their splitting and integration to be? How many peaks would you expect to find in the  $^{13}\text{C}$  NMR spectrum? What characteristic peaks would you find in the infrared spectrum?

a) 2-butanone

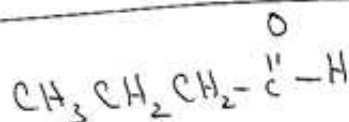


The 4 carbons are unique & give rise to 4 different  $^{13}\text{C}$  signals. The  $\text{H}_1$  and  $\text{H}_2$  protons, being adjacent to  $-\text{C}=\text{O}$  group, appear at  $\delta \approx 2$  ppm. The  $-\text{CH}_2-$  protons are split into a quartet by  $-\text{CH}_3$  group. The  $-\text{C}=\text{O}-\text{CH}_3$  protons are a ~~doublet~~ singlet.

The  $-\overset{\text{O}}{\parallel}{\text{C}}-$  at is a strong band in IR about  $1700 \text{ cm}^{-1}$ .

$\overset{\text{C}}{\text{H}} \approx 17000$

b) butanal



Again 4 carbons are unique & provide 4 diff  $^{13}\text{C}$  signals. The  $^1\text{H}$  NMR signal from  $-\overset{\text{O}}{\parallel}{\text{C}}-\text{H}$  is about  $\delta \approx 9$  ppm & a singlet. The  $-\text{CH}_2-\overset{\text{O}}{\parallel}{\text{C}}$  protons appear about  $\delta \approx 2$  ppm & are a triplet. Remaining  $\text{CH}_3\text{CH}_2-$  protons are in aliphatic region & have complex splitting.

The  $-\overset{\text{O}}{\parallel}{\text{C}}-\text{H}$  at is strong in IR about  $1750 \text{ cm}^{-1}$

4C

3H, t

2H, q

3H, s

3H, t

2H, m

2H, t

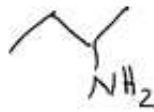
1H, s

4C

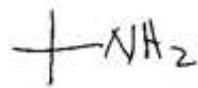
C=O

c) *s*-butylamine and *t*-butylamine

Again NMR works

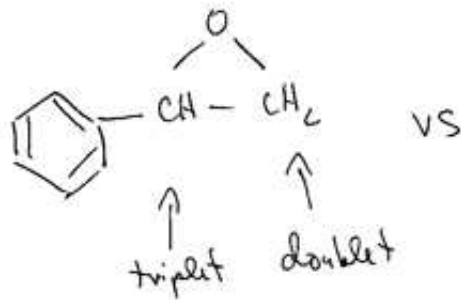


4 diff  $^{13}\text{C}$  peaks



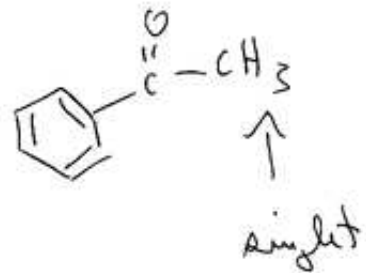
2 diff  $^{13}\text{C}$  peaks

d) styrene oxide ( $\text{C}_6\text{H}_5\text{CHCH}_2\text{O}$ ) and acetophenone ( $\text{C}_6\text{H}_5\text{COCH}_3$ )



NMR

IR



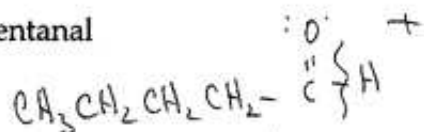
strong  $\text{C}=\text{O}$  band  
about  $1720\text{ cm}^{-1}$

W/diagram structure -2  
good method, but explanation -2  
right method 1/5

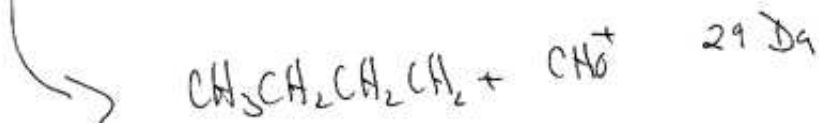
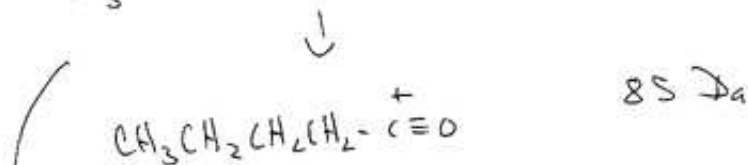


9. (10 pts) Predict the mass of the parent ion and the major mass spectral fragments to be expected for each of the following compounds.

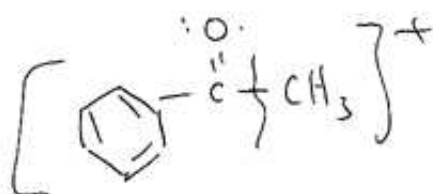
a) pentanal



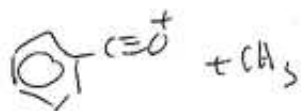
$$m/z = 86 \text{ Da}$$



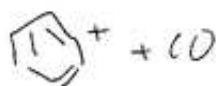
b) acetophenone ( $\text{C}_6\text{H}_5\text{COCH}_3$ )



$$m/z = 120 \text{ Da}$$



$$m/z = 105 \text{ Da}$$



$$m/z = 77 \text{ Da}$$