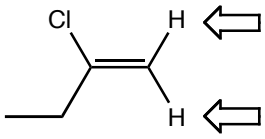
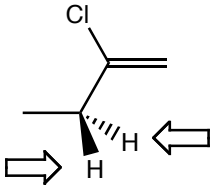
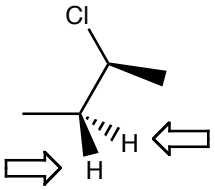
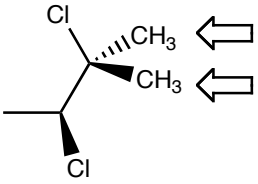
Name _____ Test 4
PHYS 0203 (Organic II) Spring 2005

1. (3 pts. each) Determine whether the indicated H atoms are diastereotopic, thus chemically inequivalent.

a. 

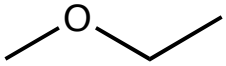
b. 

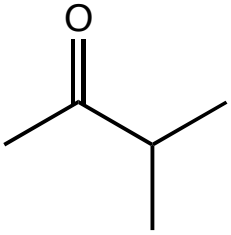
c. 

d. 

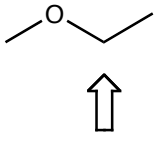
1. _____
2. _____
3. _____
4. _____
5. _____
6. _____
7. _____

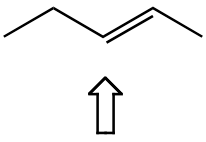
2. For the following molecules, (a. 4 pts. each) indicate the number of peaks that you expect to observe in the ^{1}H NMR spectrum, (b. 4 pts. each) indicate their relative positions (label each chemically inequivalent H with a letter. Use the letter "a" for the peak that is furthest upfield and label the rest alphabetically in order of increasing chemical shift), and (c. 4 pts each) indicate the relative areas (the integration) of each peak.

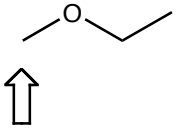
i. 

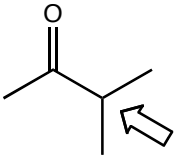
ii. 

3. (3 pts each) Determine the multiplicity of the resonance peaks attributed to the indicated proton(s).

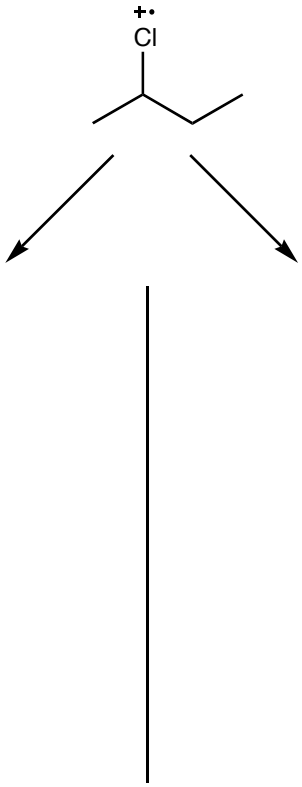
a. 

b. 

c. 

d. 

4. (10 pts) When 2-chlorobutane is converted to a cation (drawn below) in a mass spectrometer it can undergo homolytic and heterolytic bond cleavage to produce molecular fragments. Draw the products from the two possible homolytic cleavages.

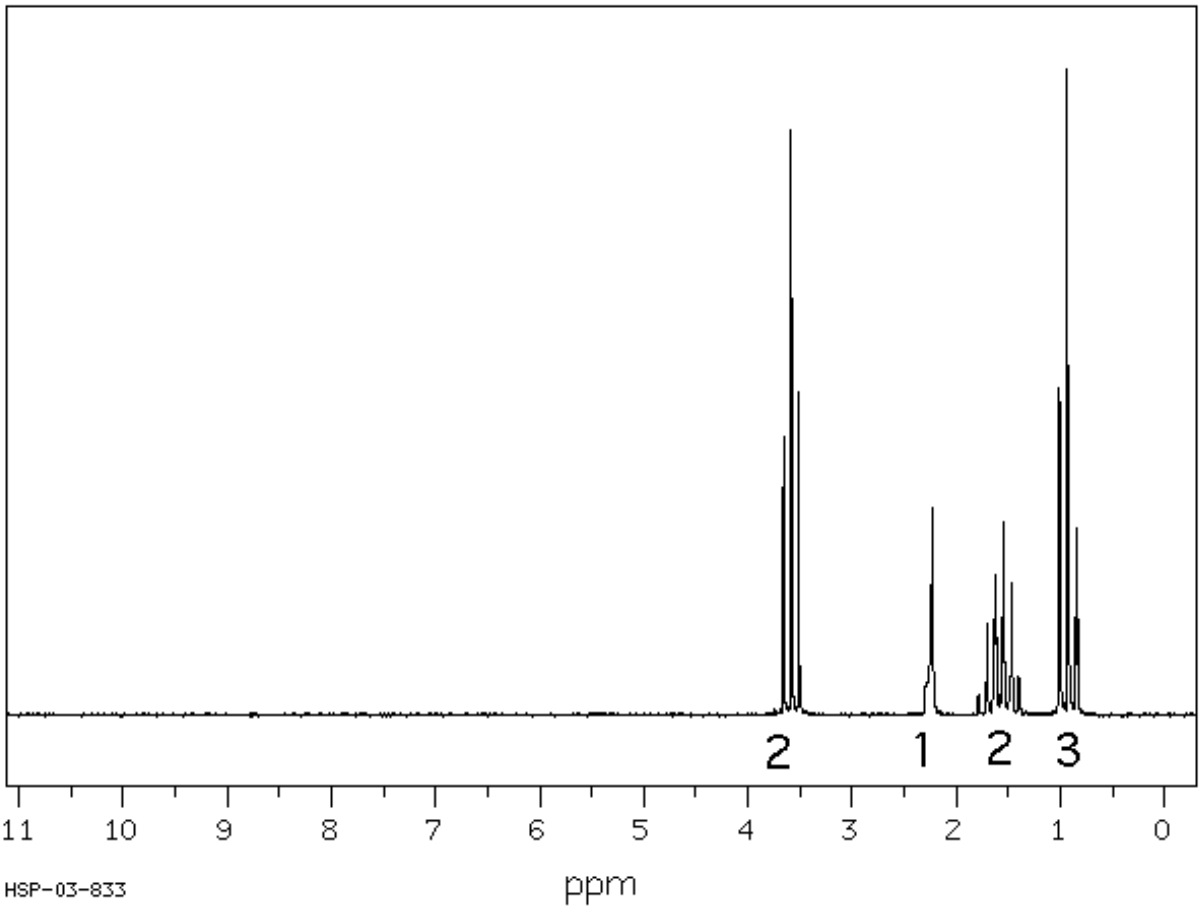


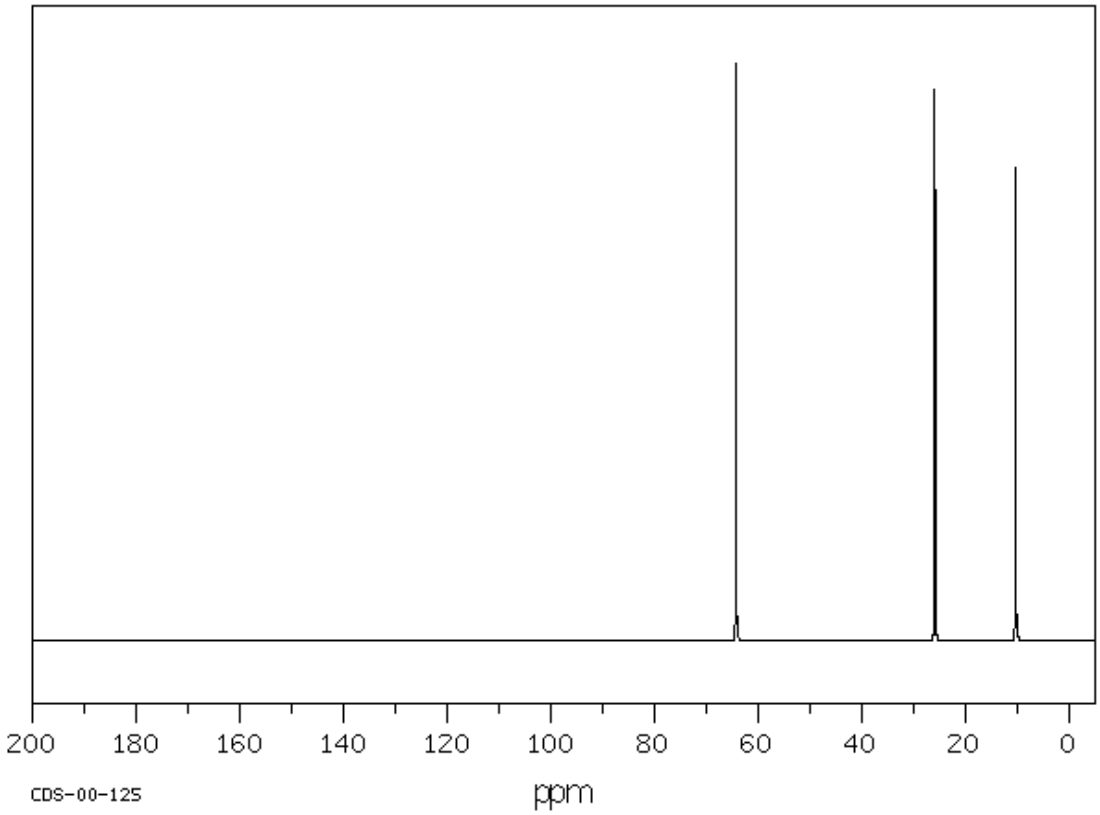
5. On the following page there is a ^{1}H NMR and a $^{13}C\{^{1}H\}$ NMR for a molecule with the formula C_3H_8O.

a. (10 pts) Determine the structure of the molecule.

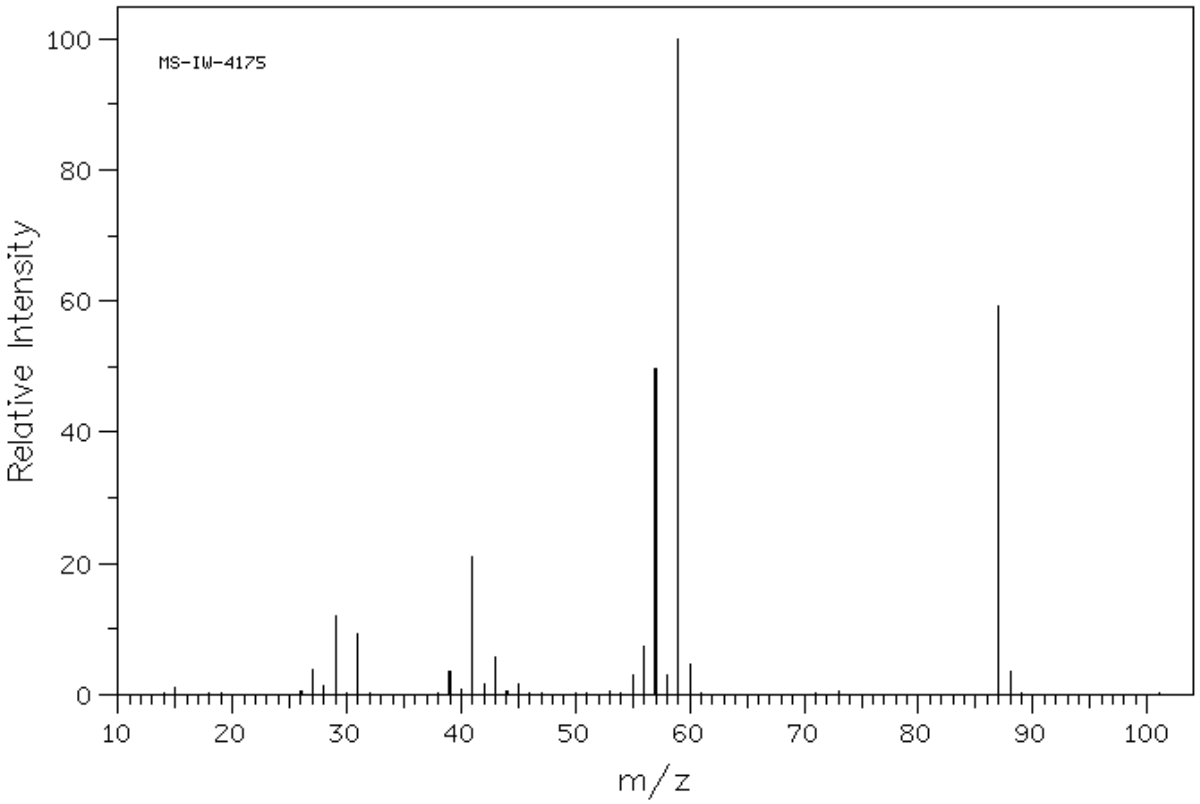
b. (4 pts) Assign the peaks in the ^{1}H NMR

c. (3 pts) Assign the peaks in the $^{13}C\{^{1}H\}$ NMR.


2
1
2
3
11
10
9
8
7
6
5
4
3
2
1
0
HSP-03-833
ppm


200
180
160
140
120
100
80
60
40
20
0
CDS-00-125
ppm

6. Below is the mass spectrum for $(CH_3)_3COCH_2CH_3$.

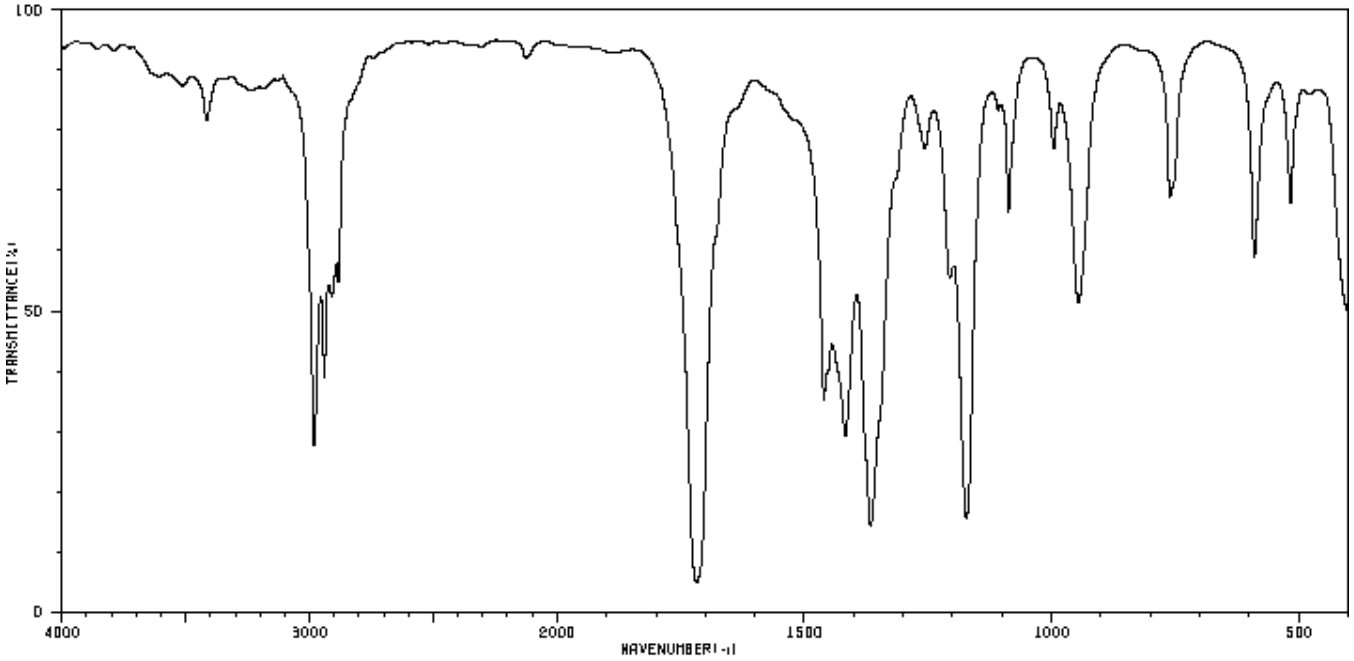


a. (6 pts) Determine the formula of the ion with an m/z ratio of 87.

b. (2 pts) To produce an ion with an m/z ratio of 87, what fragment must be lost from the parent ion?

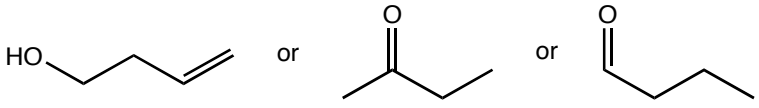
c. (6 pts) Determine the two structures that could be the ions with an m/z ratio of 87.

7. The formula for the molecule that produced the following IR spectrum is C_4H_8O.



3611	84	1718	4	1173	14
3416	79	1461	34	1087	64
2981	26	1454	36	996	74
2964	44	1417	27	946	49
2940	37	1366	13	761	66
2909	50	1257	74	590	57
2883	62	1206	69	617	66

(12 pts) Which molecule is it?



Explain your choice.