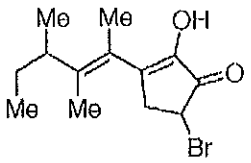
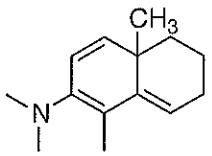
1. Calculate the UV maximum for the following compounds. Show your work as illustrated by the example below (15 points)



EXAMPLE of answer format

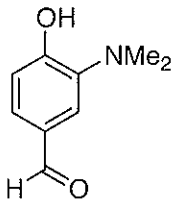
base value	202
increments for:	
double bond extending conjugation	30
alkyl substitutent or ring residues	66
polar groups	35
exocyclic double bond	none
homodiene component	none
total	333

a



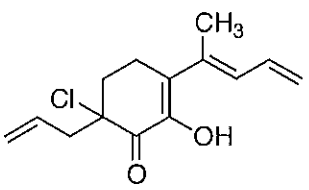
base value	253
increments for:	
double bond extenstions.	30
alkyl substitutent or ring residues	20
exocyclic double bond	5
polar groups	60
total	368

b



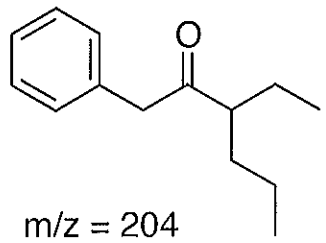
base value	250
increments for:	
alkyl or ring residue...	
–OH, –OCH_3, –OAlk..	25
$–O^-$ (oxyanion).....	
–Cl	
–Br	
$–NH_2$	
$–NHCOCH_3$.....	
$–NHCH_3$.....	
$–N(CH_3)_2$.....	20
total	295

c



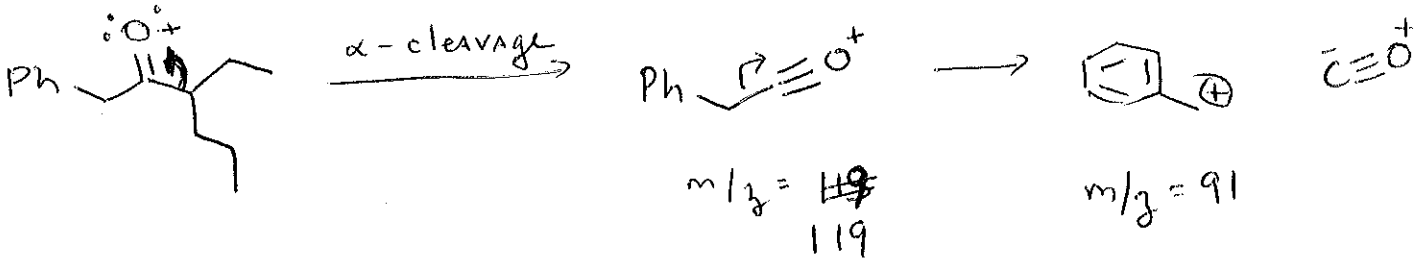
base value	215
increments for:	
double bond extending conjugation	60
alkyl substitutent or ring residues	30 (12+18)
polar groups	35
exocyclic double bond	
homodiene component	
total	340

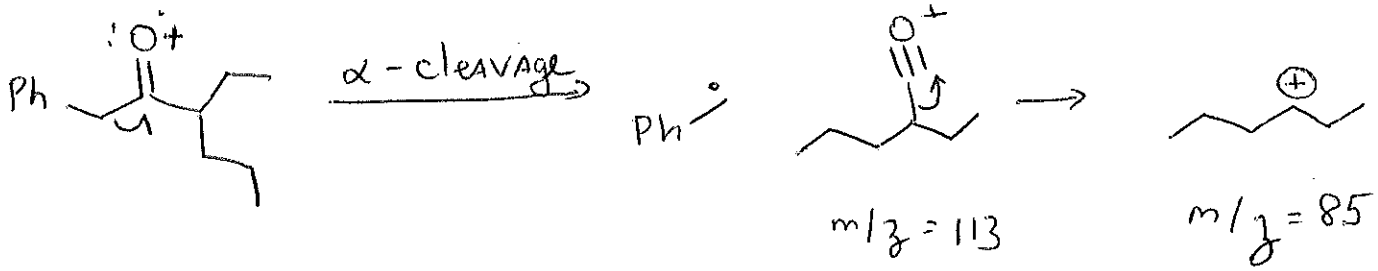
2. Explain how the indicated fragments are formed. Your answer should provide both a chemical structure and a mechanism for the formation of each fragment peak.

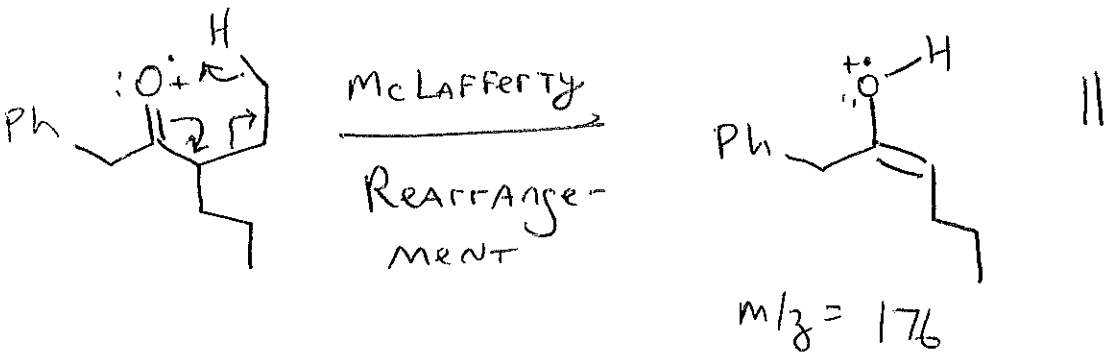


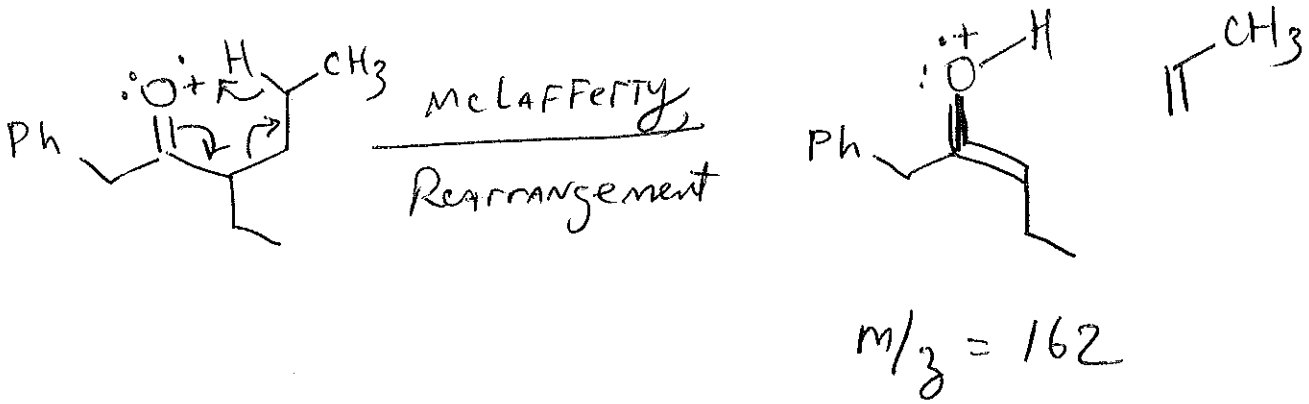
m/z = 204

m/z = 85
m/z = 91
m/z = 113
m/z = 119
m/z = 162
m/z = 176

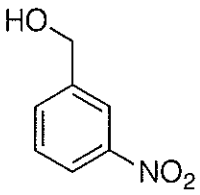




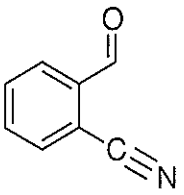




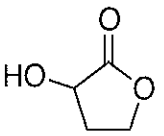
3. Match the following to their IR spectra. Note, only 4 spectra have a match. (16 points)



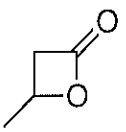
A



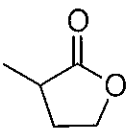
B



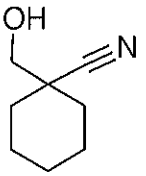
C



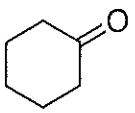
D



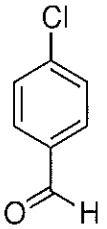
E



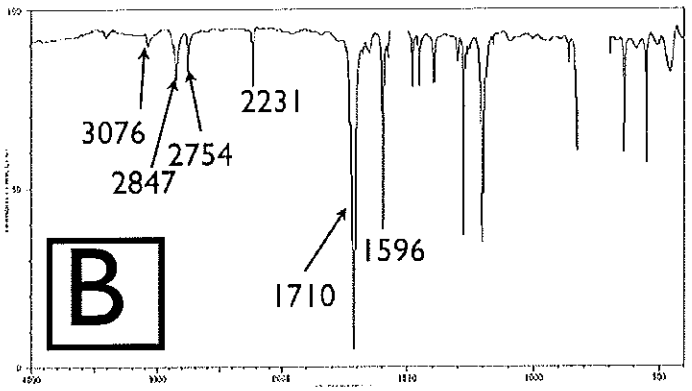
F

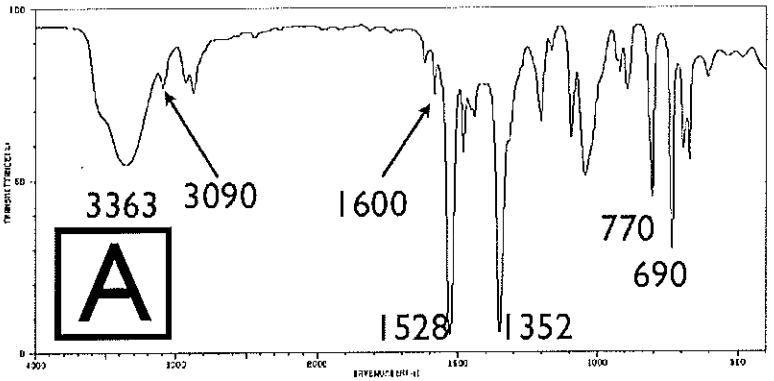


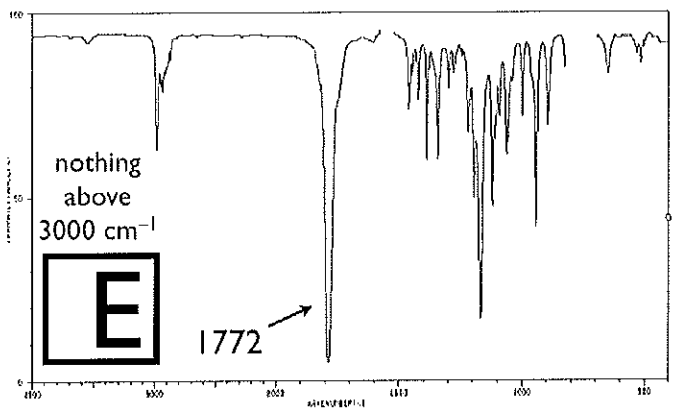
G

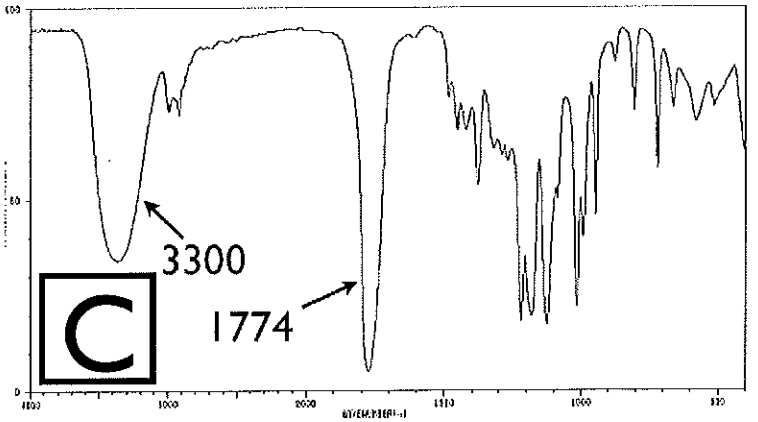


H









4. Elucidate the following structure based on the following spectral data

$C_{12}H_{20}O$

^{1}H NMR
5.77 (ddt, J = 17.0, 10.0, 7.0 Hz, 1H)
5.01 (ddt, J = 17.0, 2.1, 1.0 Hz, 1H)
4.97 (ddt, J = 10.0, 2.1, 1.2 Hz, 1H)
2.56 (ddd, J = 12.5, 11.5, 4.0 Hz, 1H)
2.32-2.17 (m, 2H)
1.96-1.90 (m, 2H)
1.87-1.83 (m, 1H)
1.56-1.38 (m, 8H)
1.02 (d, J = 7.0 Hz, 3H)

^{13}C NMR
215, s
138, d
115, t
55, d
42, t
36, d
35, t
32, t
30, t
28, t
26, t
21, q

IR (cm^{-1}, neat) : 3079, 2936, 1706, 1640, 1450, 1325, 1248, 998, 915

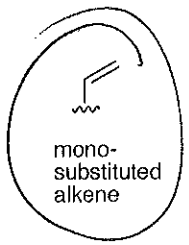
MS 180 (M+, parent peak), 126, 41

a) Calculate the IHD: 3 (1 point)

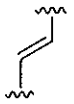
b) How many hydrogens are on carbons? 20 (1 point)

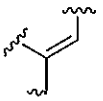
c) Show the substructure that is associated with the following IR peaks (4 points)

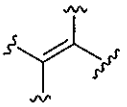
3079 cm $^{-1}$, 1640 cm^{-1}


mono-substituted alkene


cis-disubstituted alkene

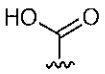

trans-disubstituted alkene

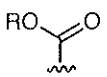

trisubstituted alkene

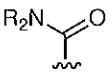

tetrasubstituted alkene


ketone


aldehyde

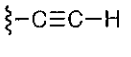

acid

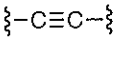

ester


amide


nitro

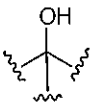

nitrile


terminal alkyne

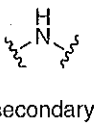

internal alkyne

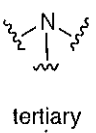

primary alcohol

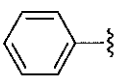

secondary alcohol

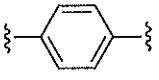

tertiary alcohol

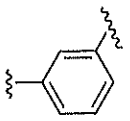

primary amine

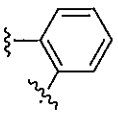

secondary amine

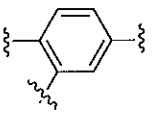

tertiary amine


monosubstituted benzene


1,4-disubstituted benzene


1,3-disubstituted benzene

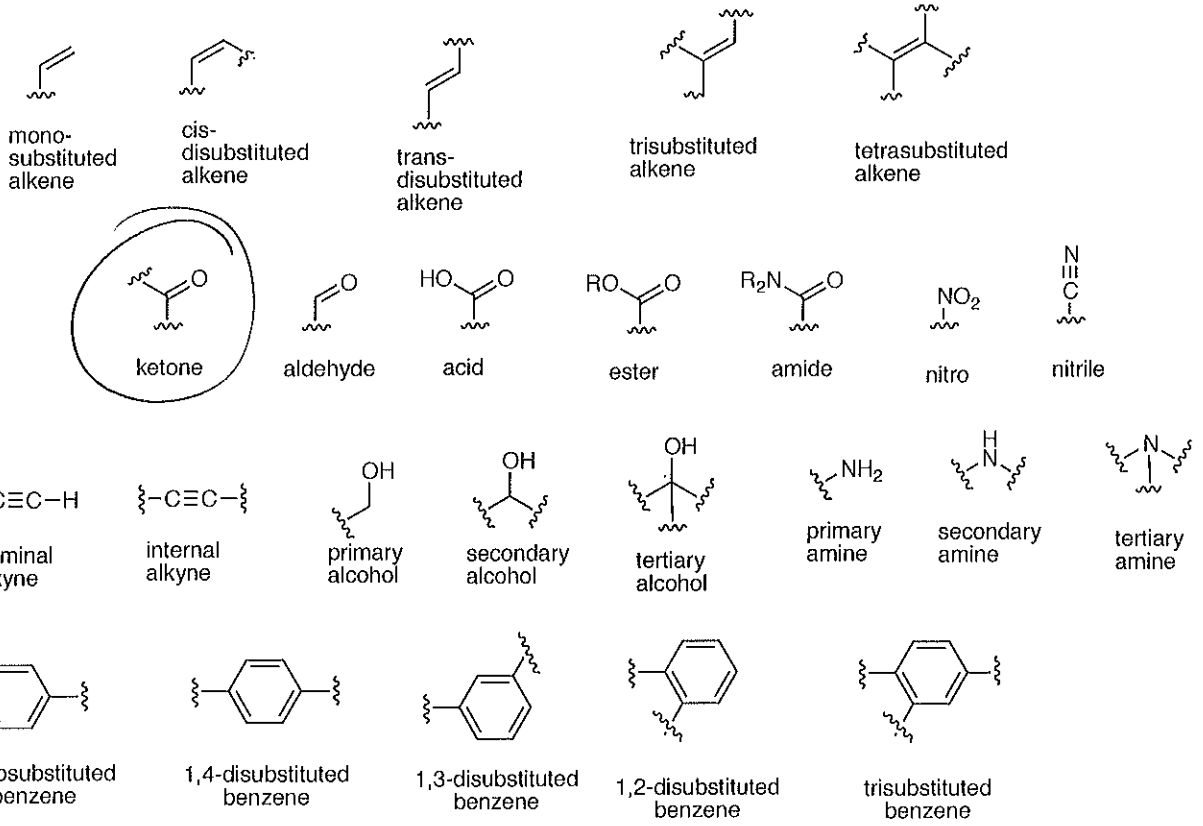

1,2-disubstituted benzene


trisubstituted benzene

none of the above

d) Show the substructure that is associated with the following IR peak (4 points).

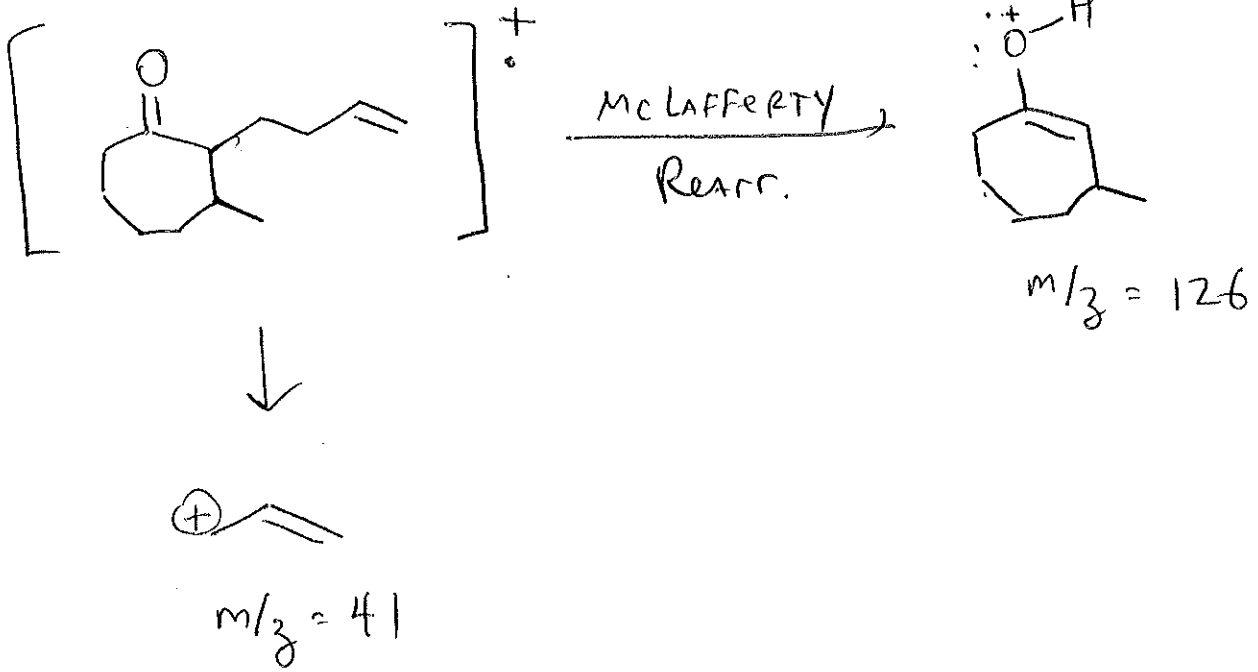
1706 cm $^{-1}$



none of the above

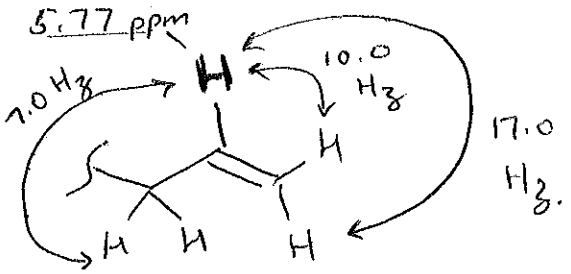
e) Assign the following mass spectral fragments (10 points). Draw the structures of the fragments.

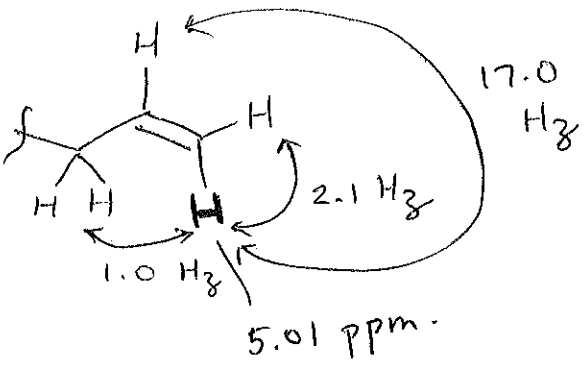
126, 41

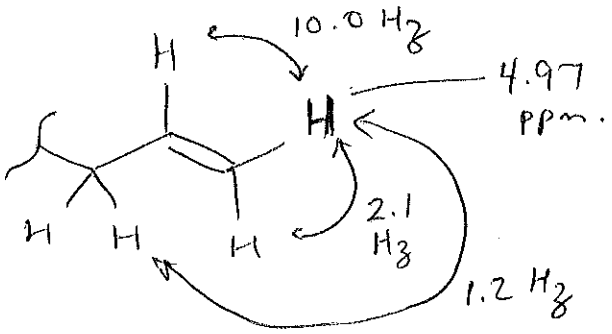


f) Show the substructure that is associated with the following ^{1}H NMR resonances. Assign the coupling constants. Also, indicate the multiplicity (s,d,t or q) of the carbon to which this substructure is attached. (8 points)

5.77 (ddt, J = 17.0, 10.0, 7.0 Hz, 1H)
5.01 (ddt, J = 17.0, 2.1, 1.0 Hz, 1H)
4.97 (ddt, J = 10.0, 2.1, 1.2 Hz, 1H)







g) Does your compound have a ring? If so, what size? Hint: pay careful attention to the IR peak at 1706 cm–1 (5 points)

circle the correct ring size

3 4 5 6 (7)

8 9 10 no ring

h) Draw the structure (12 points)