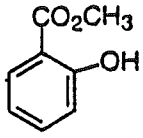
CHEMISTRY 744

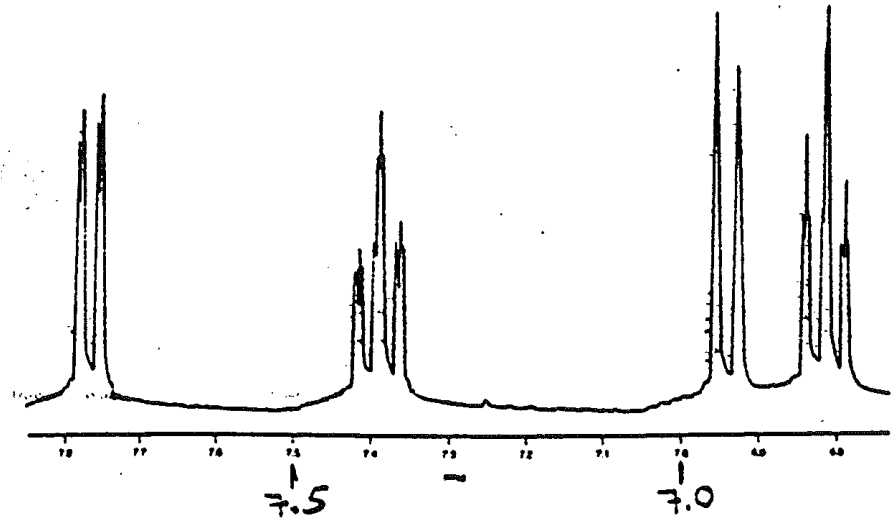
Organic Spectroscopy, Fall 2015

Homework #3

due Thursday, October 1

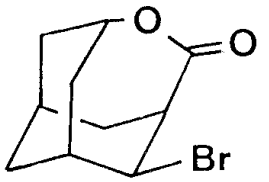
1. The following set of spectra shows the ^{1}H aromatic region expansion for methyl salicylate, and a HETCOR spectrum. The HETCOR only shows carbons that have protons attached. Assign all the protons and carbons shown on the HETCOR to the structure. Include an assignment for proton resonances at 3.8 and 10.6 ppm.





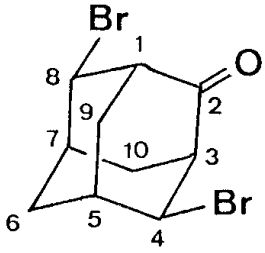
2. (C) The hydrobromic acid catalyzed rearrangement of the bromolactone **4** resulted in the three isomeric dibromoadamantanones **5**-**7**. Examine the following NMR data and assign the correct structure to this data.

^{1}H NMR

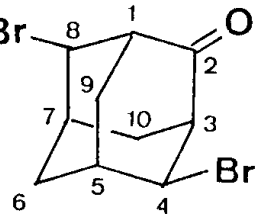


4

HBr

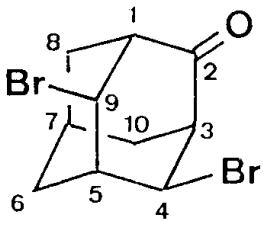


+

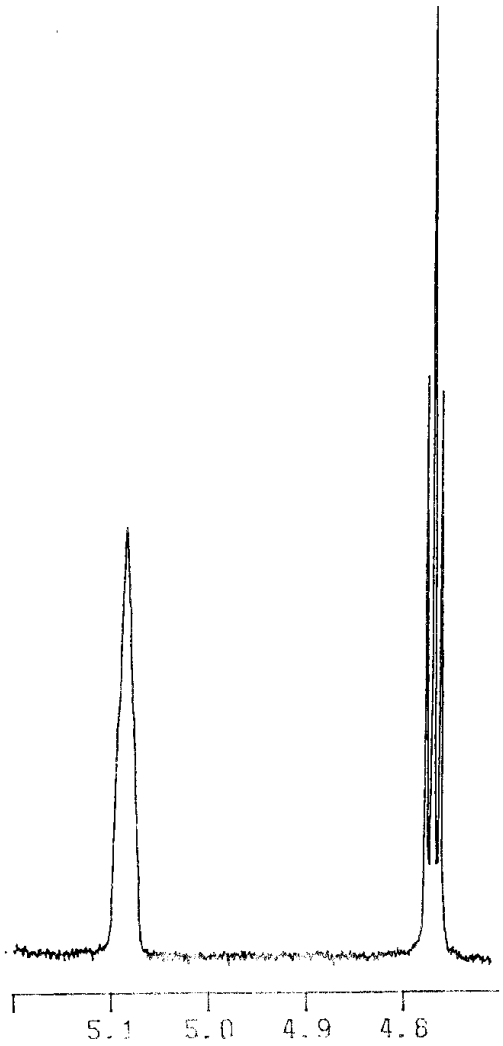


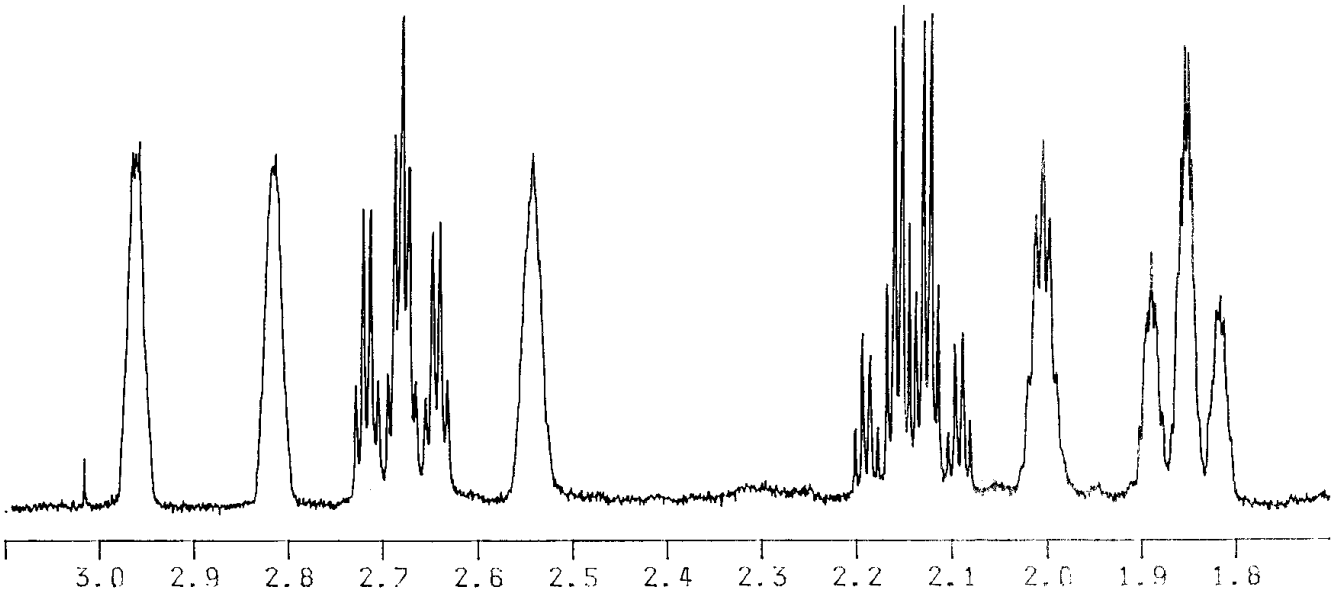
5 6

+

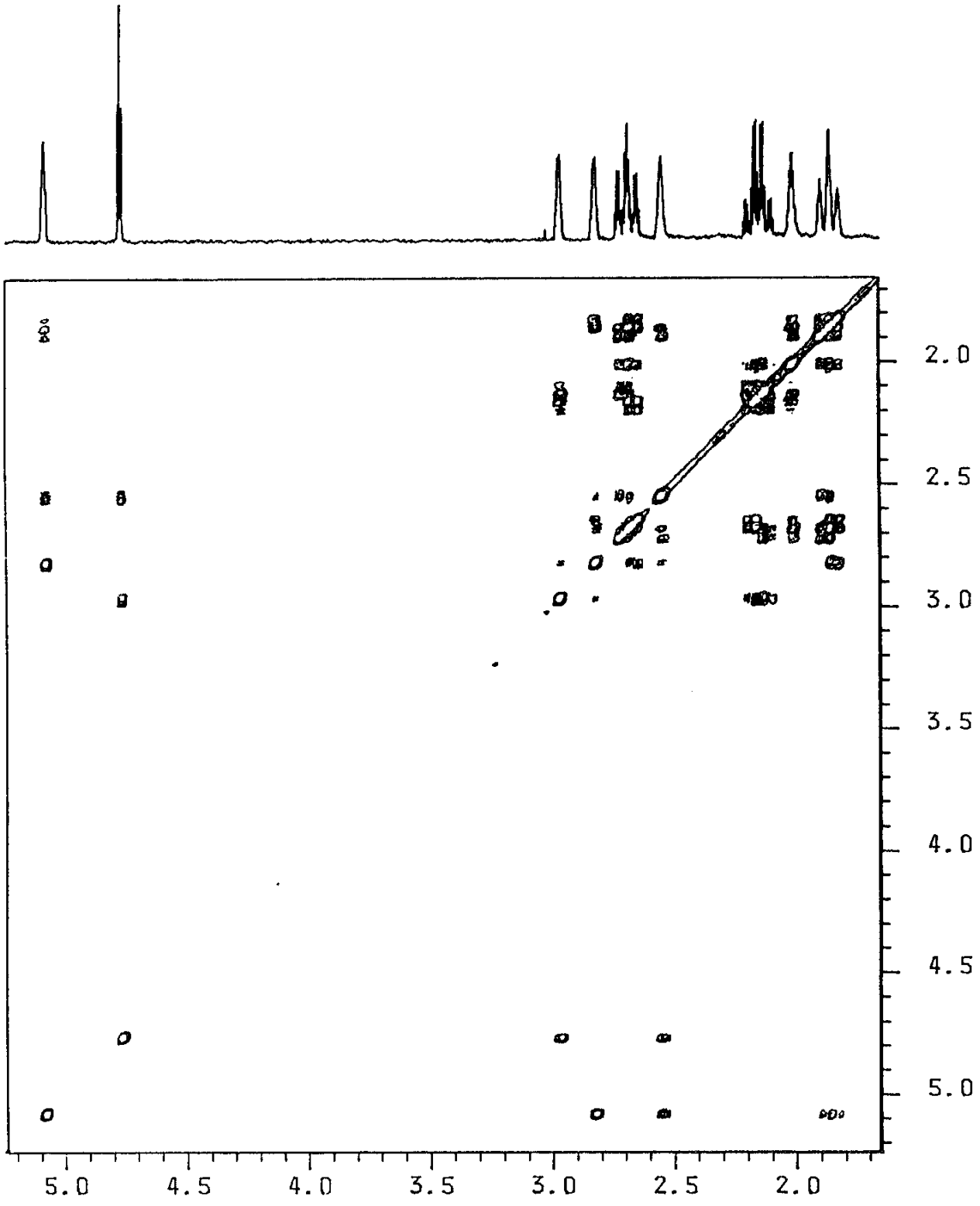


7

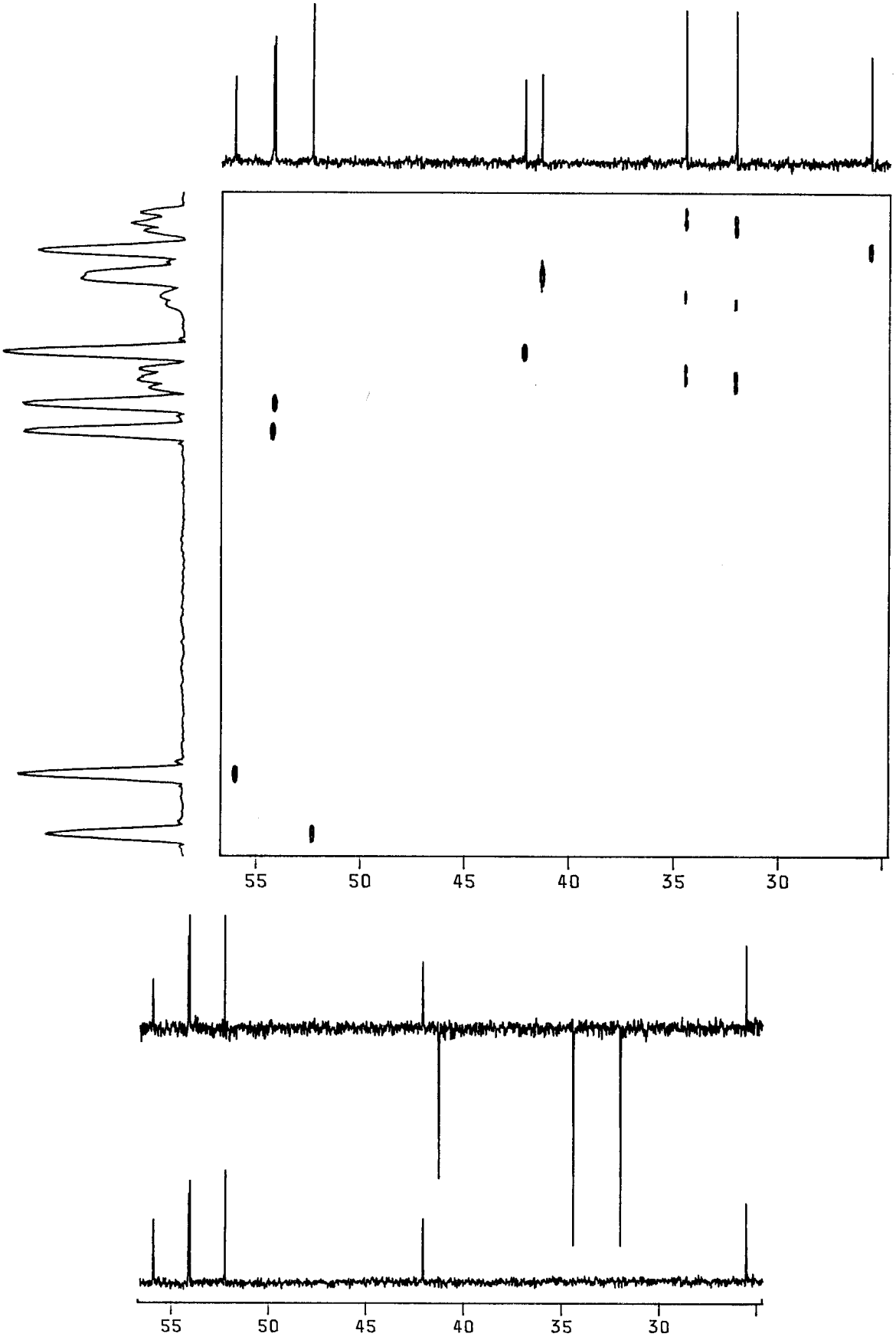




^{1}H-^{1}H COSY

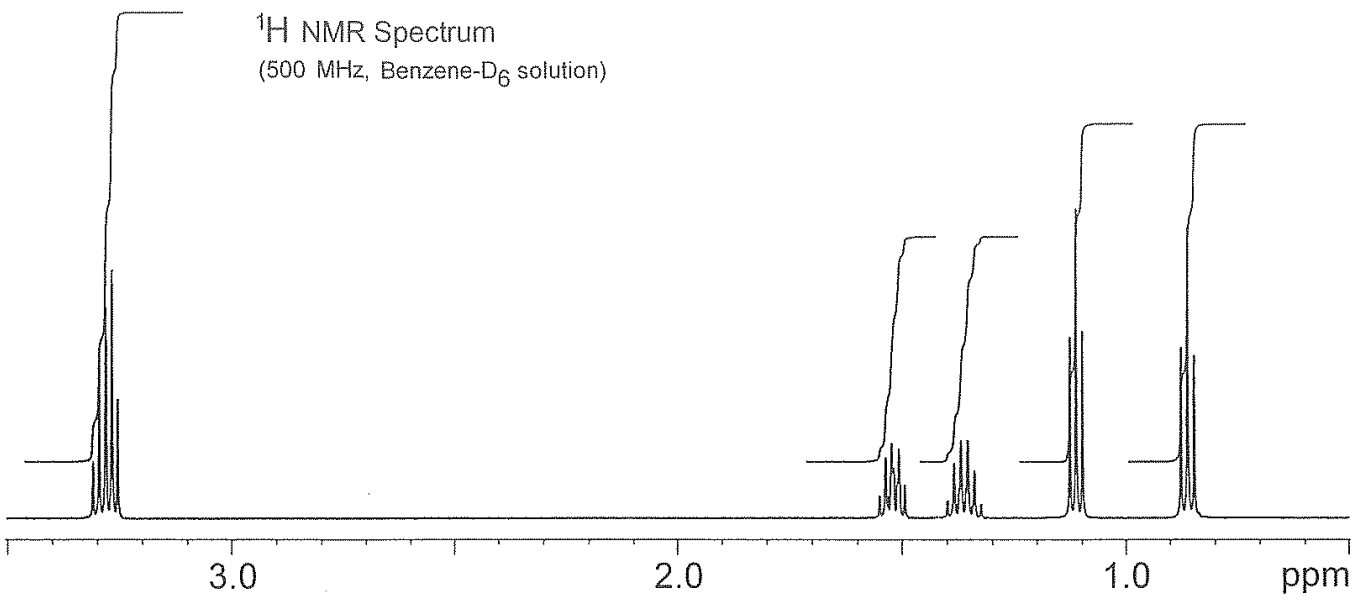


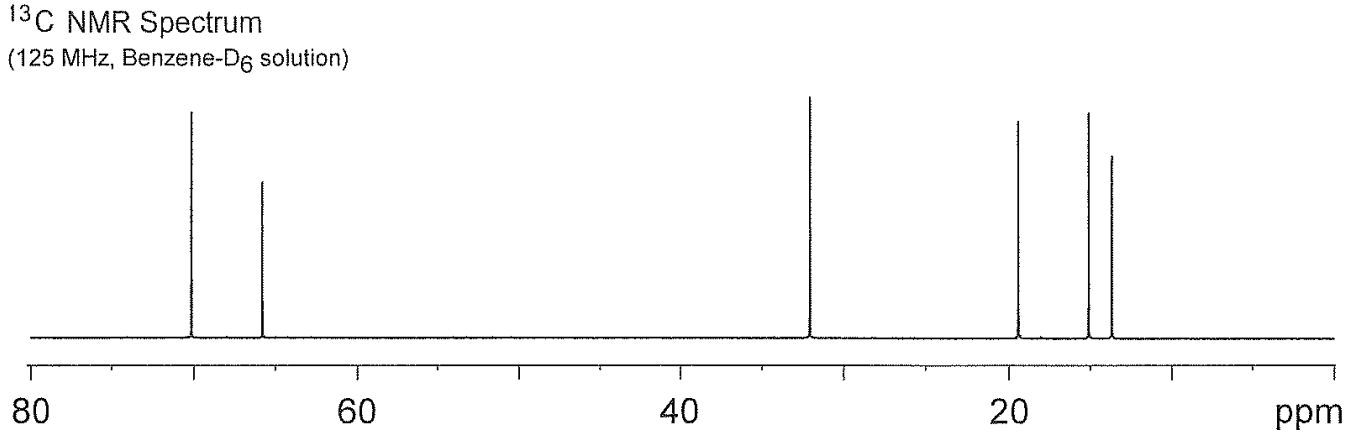
^{1}H-^{13}C COSY (HETCOR) and DEPT

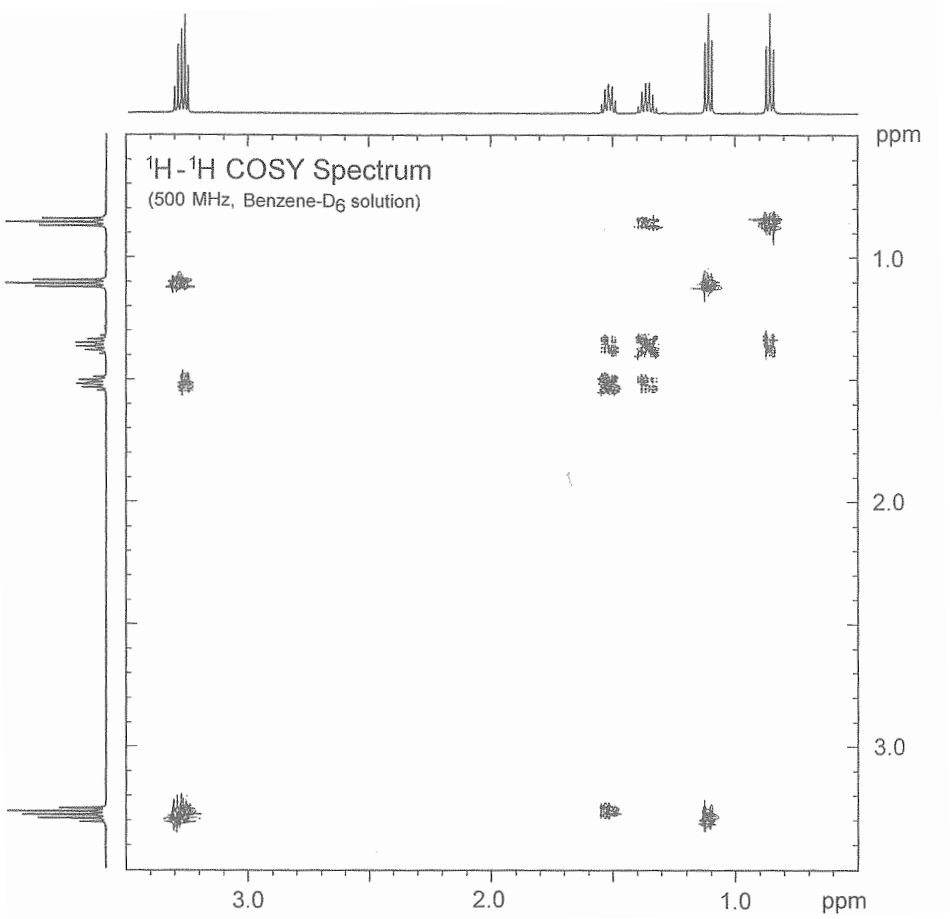


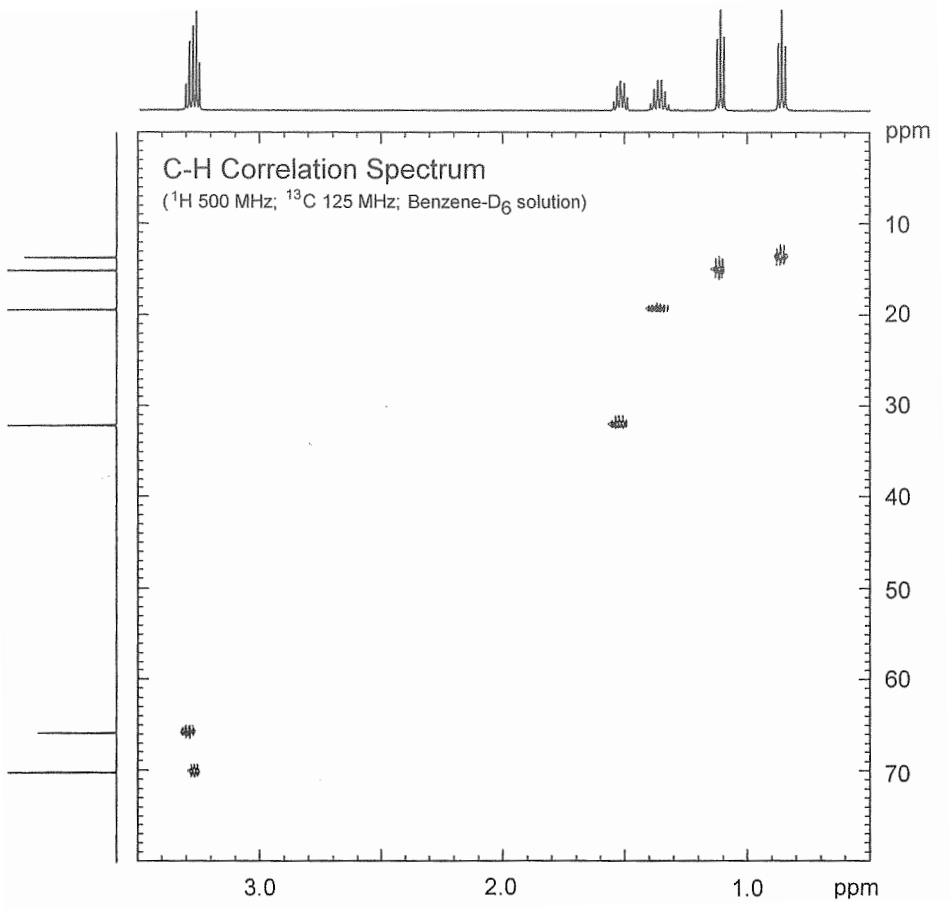
DEPT bottom: CH; top: CH, CH_3 up, CH_2 down

3. The NMR data below (proton, carbon, COSY, HETCOR) is for an unknown compound with a molecular formula of $C_6H_{14}O$. Determine the structure and assign all proton and carbon resonances to the structure.






^{1}H-^{1}H COSY Spectrum
(500 MHz, Benzene-D$_6$ solution)
ppm
1.0
2.0
3.0
3.0
2.0
1.0
ppm


C-H Correlation Spectrum
(^{1}H 500 MHz; ^{13}C 125 MHz; Benzene-D$_6$ solution)
ppm
10
20
30
40
50
60
70
3.0
2.0
1.0
ppm