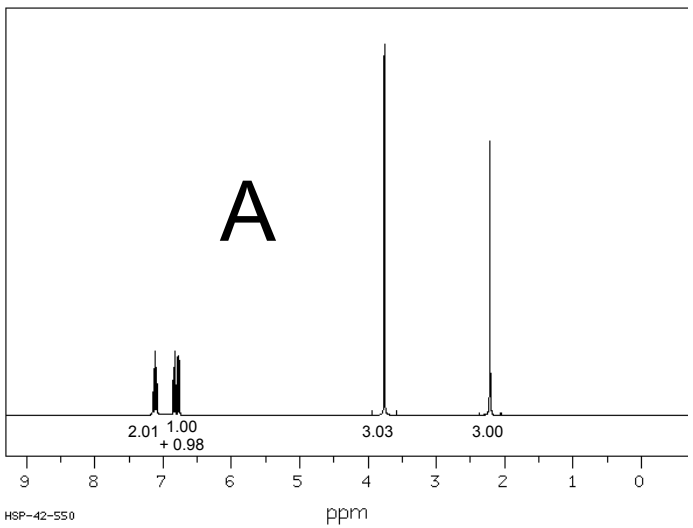
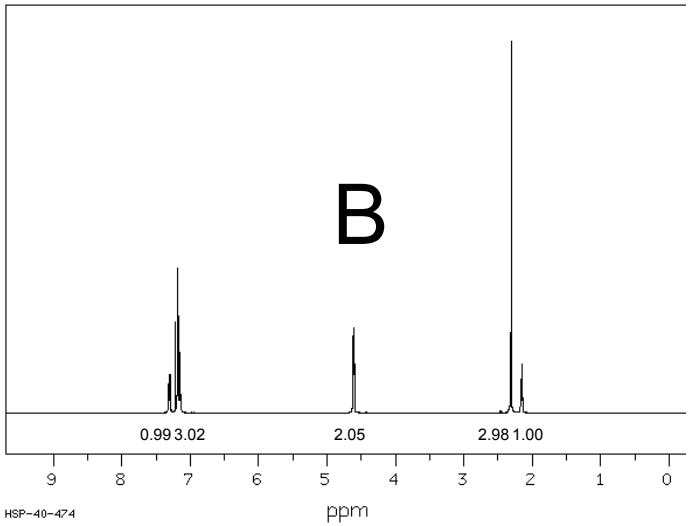
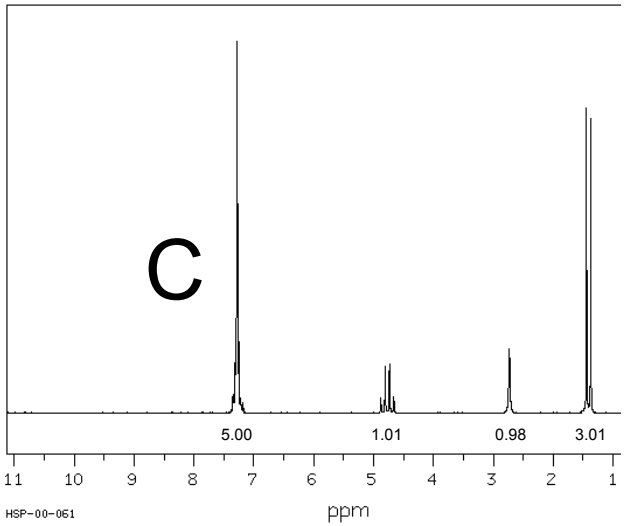
CHEM 3201 Midterm Examination II, November 26, 2010 120 Minutes Total Marks = 100

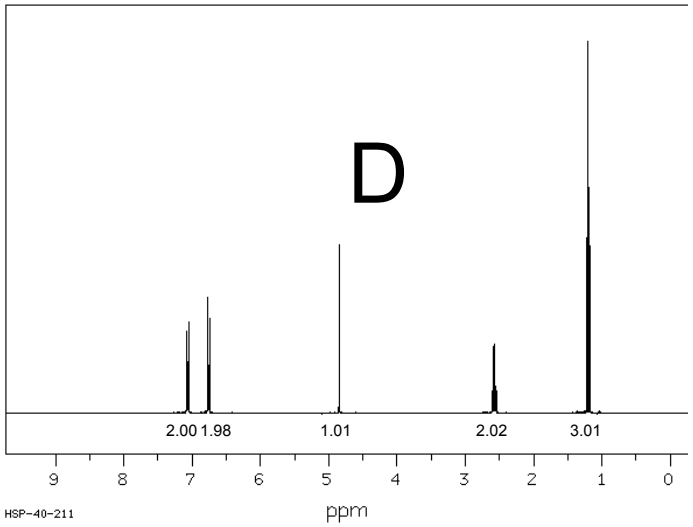
You may use your textbook, a molecular model kit, a calculator and a ruler.

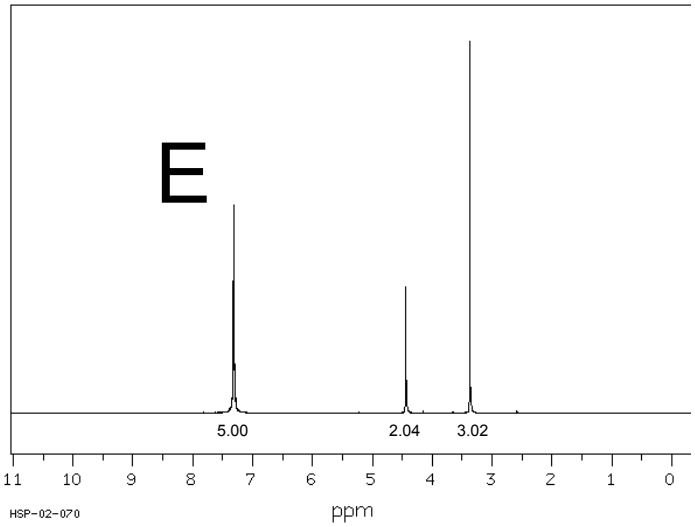
1. The following proton spectra are isomers of **$C_8H_{10}O$**. Provide the correct structure for each spectrum. **30 marks**

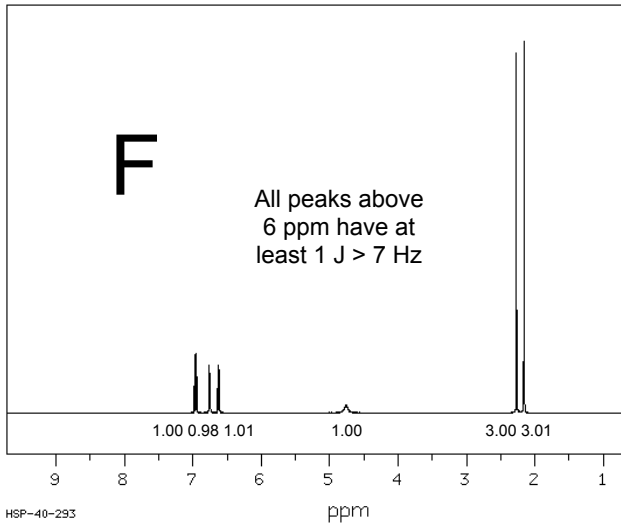






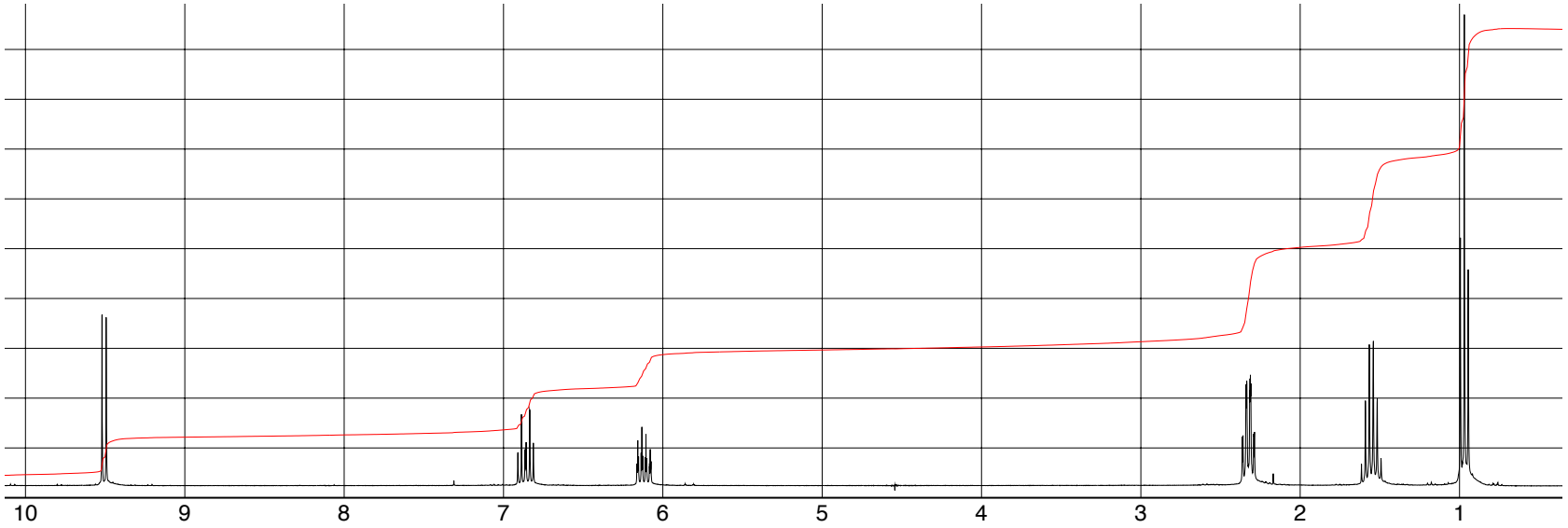




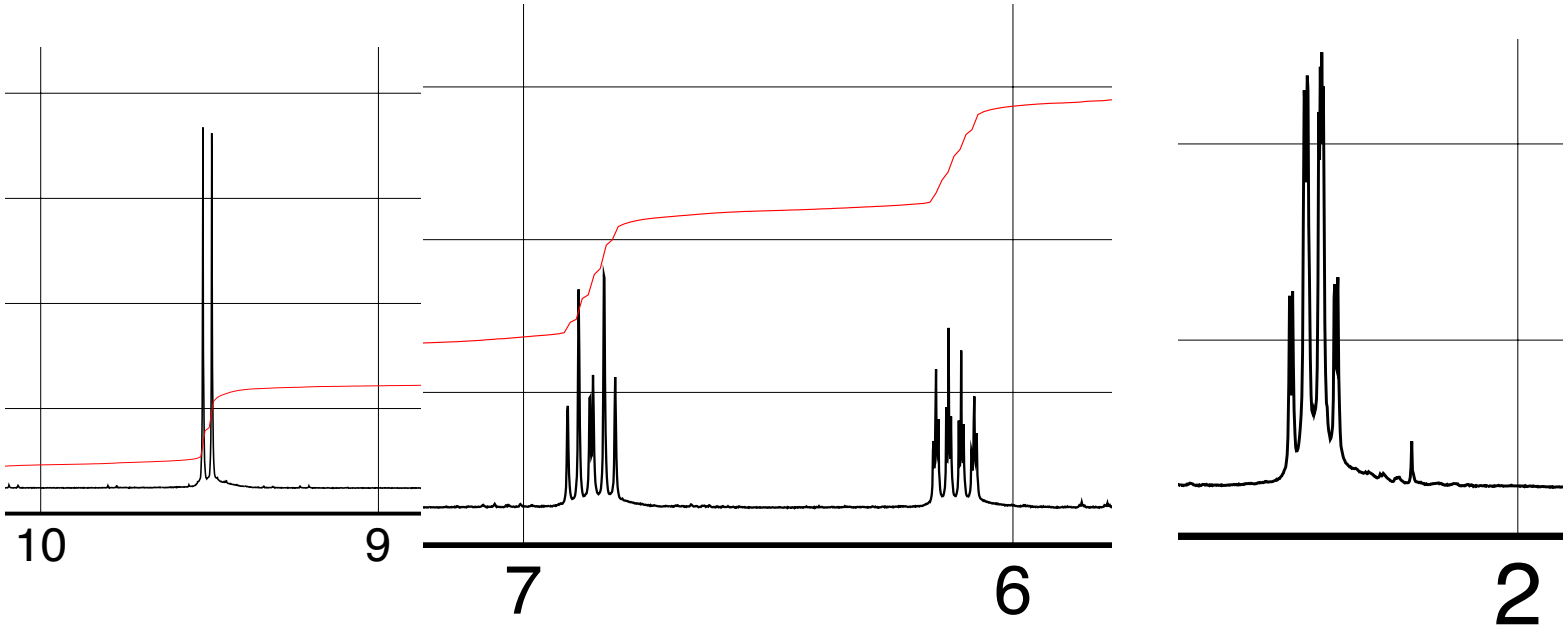


2. a) Use the provided graph paper to draw a doublet of quartets with *J* values of 7 and 2 Hz.
b) Draw a quartet of doublets with *J* values of 7 and 2 Hz on the graph paper. Indicate the line intensities in each case. **10 marks**

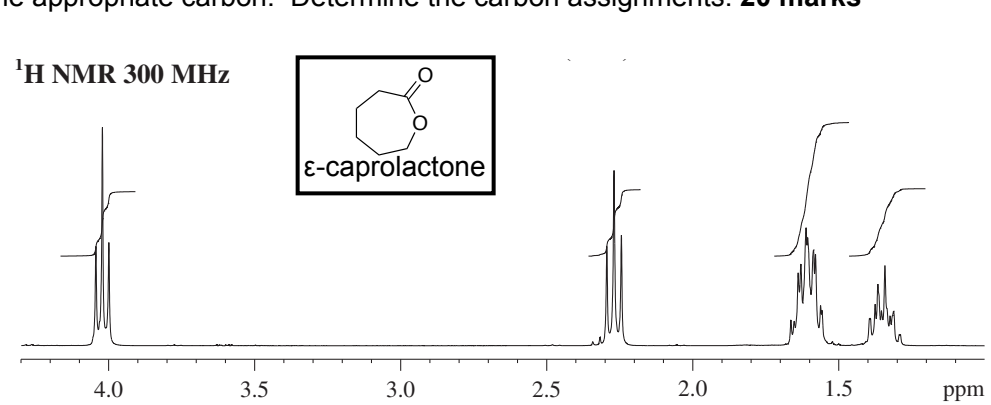
3. The 300 MHz ^{1}H NMR spectrum for 2-hexenal is presented below (with some expansions). The peak data for peaks above 6.0 ppm is also given.
a) For the peaks between 6 and 7 ppm, extract the coupling constants and explain their origin (^{2}J, ^{3}J, *etc.*). **10 marks**
b) Is this a spectrum of *E*-2-hexanal or *Z*-2-hexanal? How do you know? **5 marks**

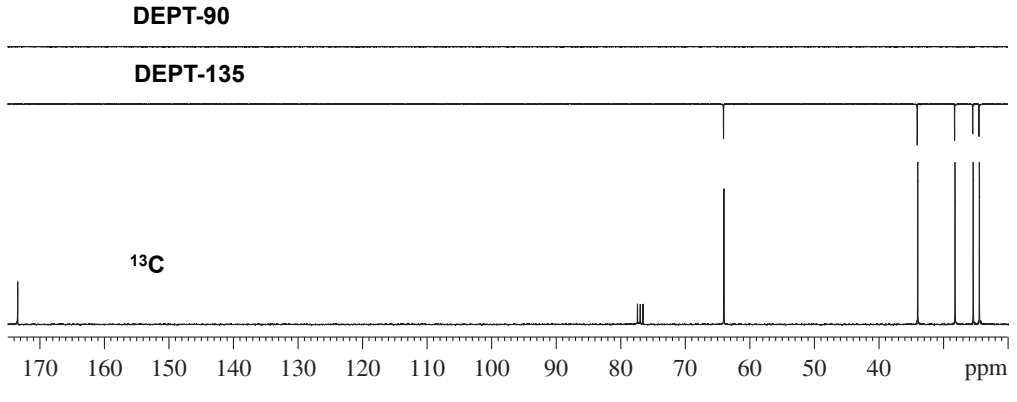


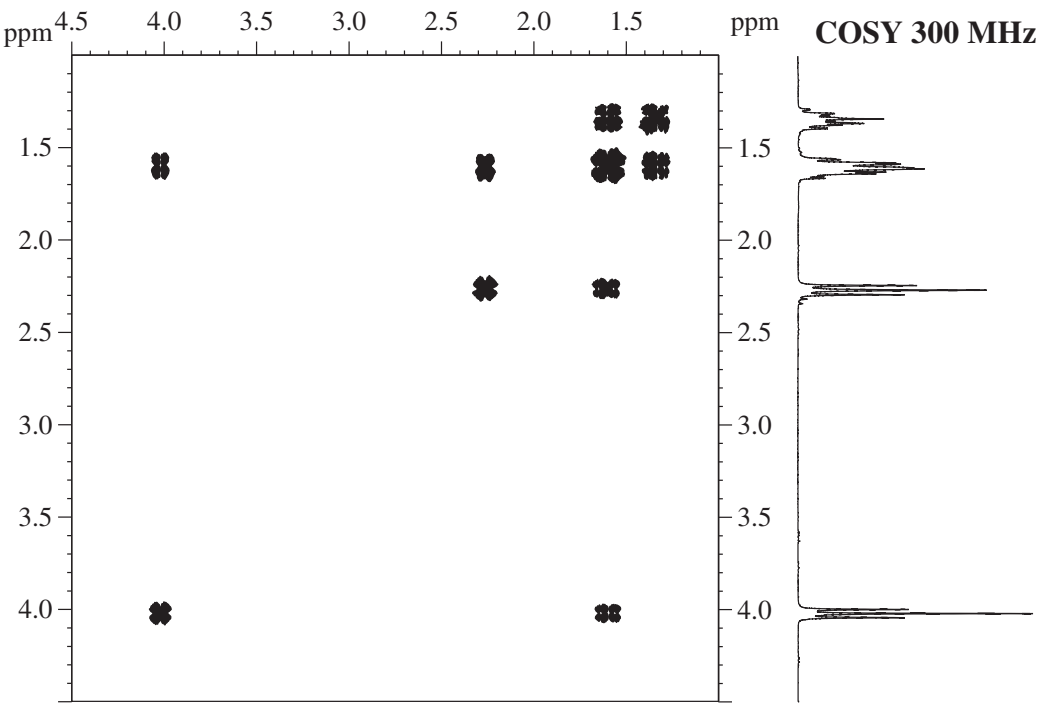
Hz	ppm
2857.15	9.524
2849.45	9.498
2069.20	6.897
2062.50	6.875
2055.80	6.853
2053.60	6.845
2046.90	6.823
2040.20	6.801
1851.45	6.172
1850.05	6.167
1848.65	6.162
1843.75	6.146
1842.35	6.141
1840.95	6.136
1835.85	6.120
1834.45	6.115
1833.05	6.110
1828.15	6.094
1826.75	6.089
1825.35	6.084

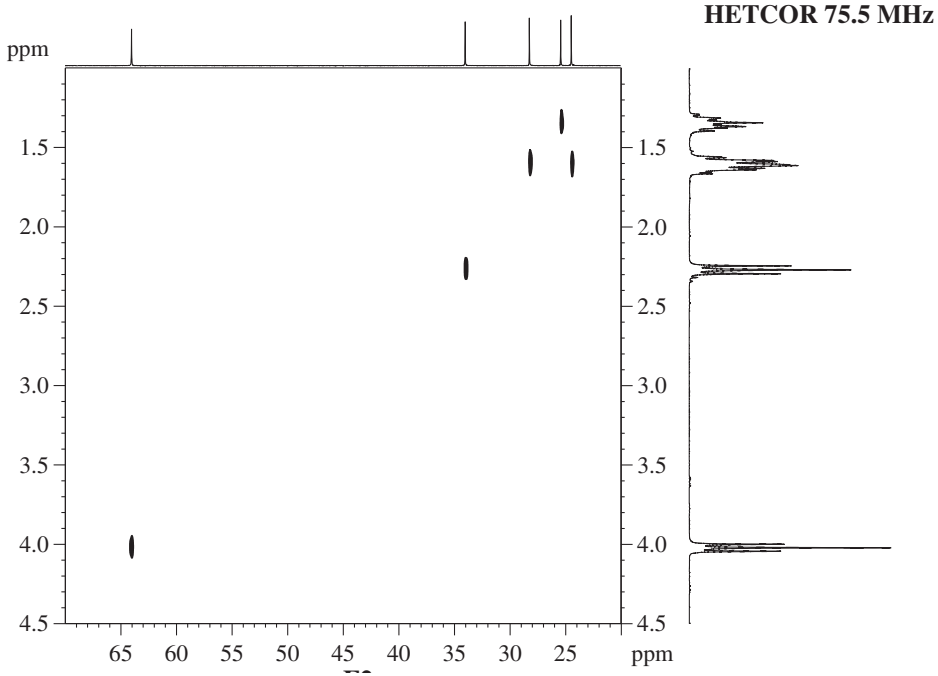


4. Given the structure of ε-caprolactone, assign all of the proton signals to the appropriate carbon. Determine the carbon assignments. **20 marks**









5. You have been given IR, ^{1}H, ^{13}C, DEPT, COSY and HMQC data for a molecule with the formula $C_7H_{14}O_2$. (a) What is the structure of the molecule? (b) Assign each proton and carbon signal to the correct proton/carbon of the structure. Include a brief explanation for your assignments. **25 marks**