ORGANIC CHEMISTRY 136

(Prof. Yves Rubin)

UCLA, SPRING 2012

MIDTERM EXAM

_____

Your name

Question	Points
1 (30)	
2 (20)	
3 (25)	
4 (25)	

Total (100)
=========

Name

1. a) (10 points) Explain using only a *few sentences and/or a diagram* why the C–H stretching frequency of $CHCl_3$ appears at 3000 cm^{-1}, while the C–D stretching frequency for $CDCl_3$ appears at 2260 cm^{-1}.

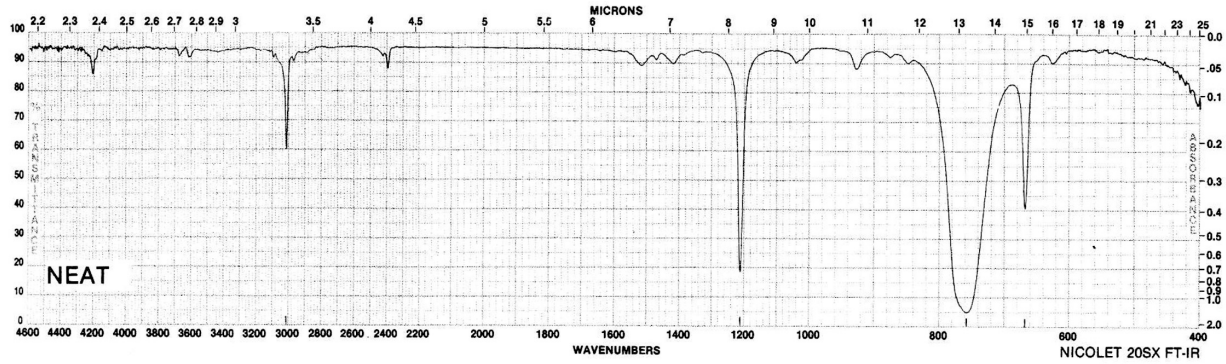


FIGURE 8.2b IR spectrum of $CHCl_3$.

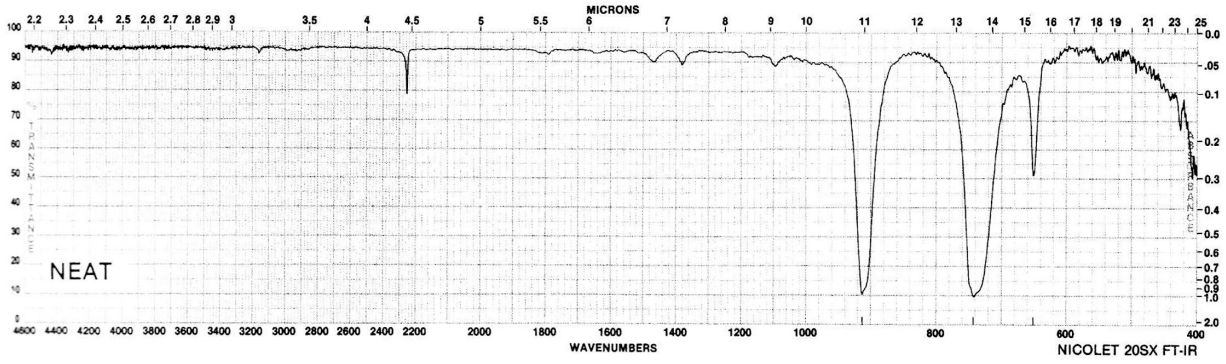


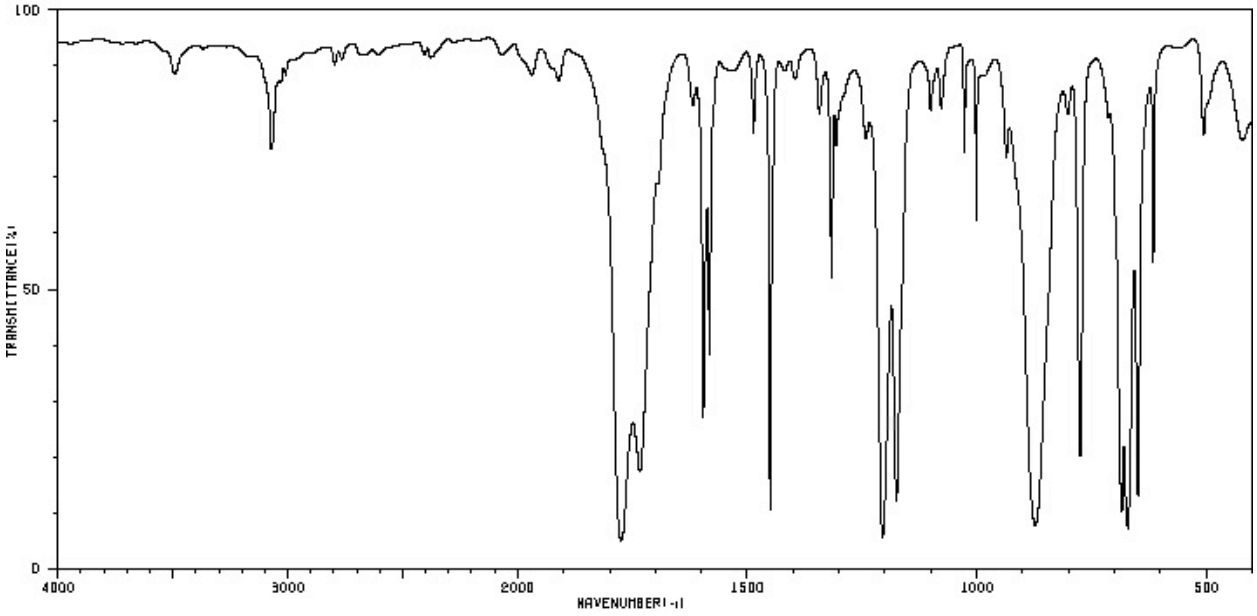
FIGURE 8.2c IR spectrum of $CDCl_3$.

Name

Question 1 continued:

b) (5 points) What are the absorption bands at 1205 and 907 cm^{-1} in the IR spectra of $CHCl_3$ and $CDCl_3$, respectively?

c) (10 points) Explain the doubled peak at 1775 and 1733 cm^{-1} in the following IR spectrum. Also, what vibration does the *associated fundamental* frequency correspond to?

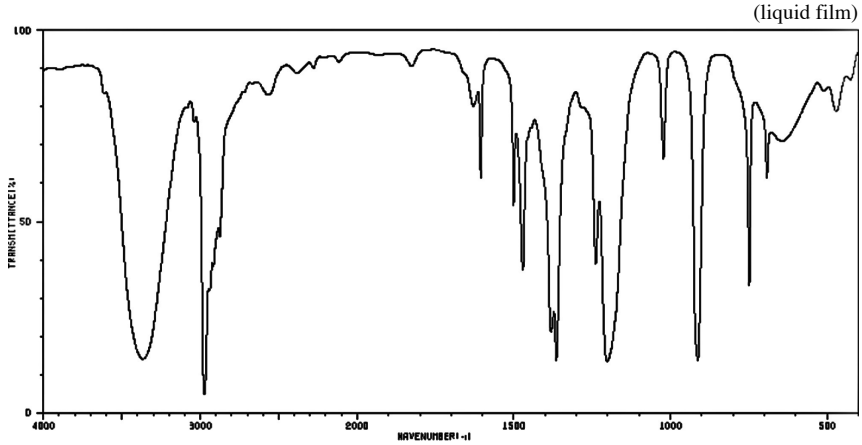


d) (5 points) Explain the absorption peak at 3470 cm^{-1} in the IR spectrum above:

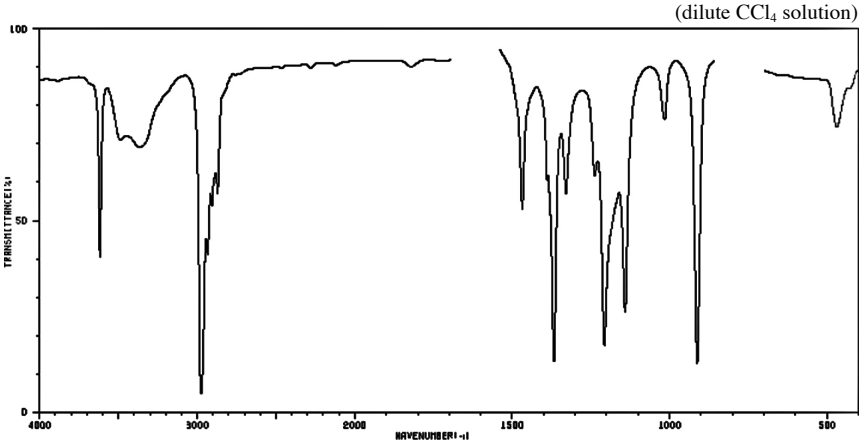
Name _____

2. a) (10 points) A compound contains 4 carbons and displays only 1 *sharp* singlet in its ^{1}H NMR spectrum along with one broad singlet. Using its IR spectra recorded in two different media (neat film or dilute CCl_4 solution), assign recognizable absorptions in both spectra, labeling clearly what type they are, and provide the structure that fits these data:

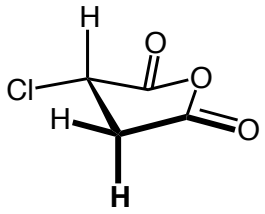
(liquid film)

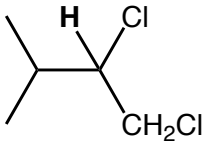


(dilute CCl_4 solution)



b) (10 points) Draw theoretical ^{1}H NMR *coupling patterns* (i.e. the way splittings would appear in a ^{1}H NMR spectrum) for the **H**'s highlighted in boldface in the following two compounds. Also label the pattern (e.g. t, dd):

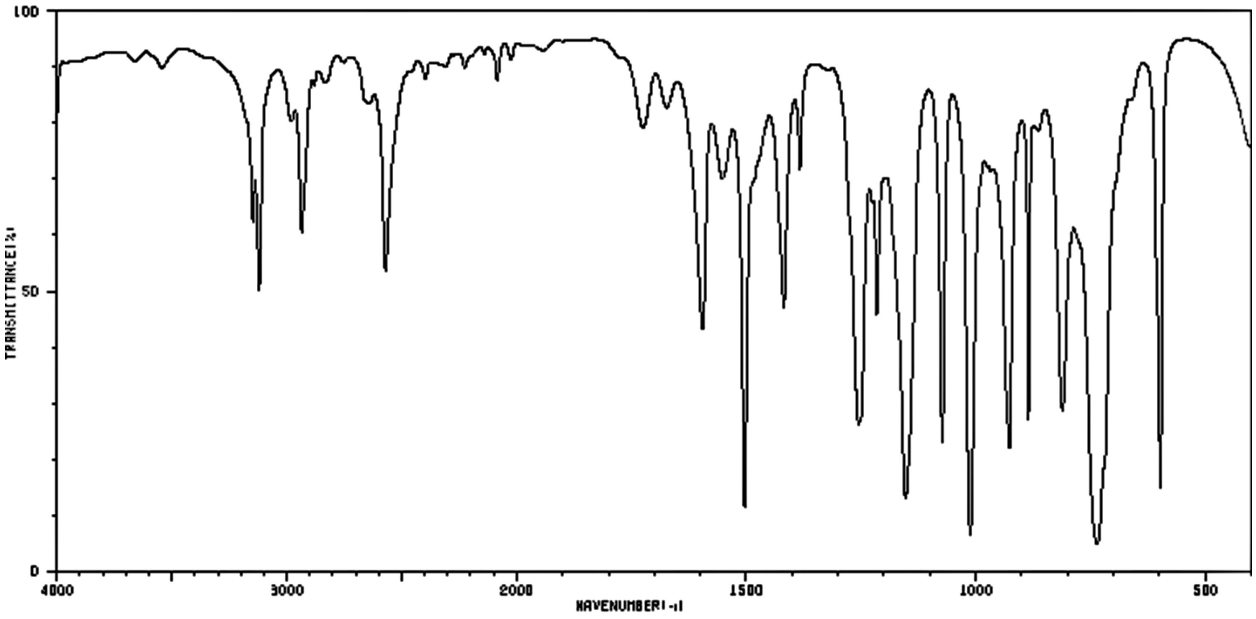




_____ _____

Name

3. a) (25 points) In addition to carbon and hydrogen atoms, the exact number of which you can determine from the ^{1}H and ^{13}C NMR spectra provided below, the following compound contains only two heteroatoms, 1 oxygen and 1 sulfur. Its IR spectrum is also provided to help you with structure determination. Assign recognizable IR absorptions, as well as *all* the signals of the ^{1}H NMR spectrum (but not carbons in this problem). Then provide the structure of this compound and provide your reasoning:



(liquid film)

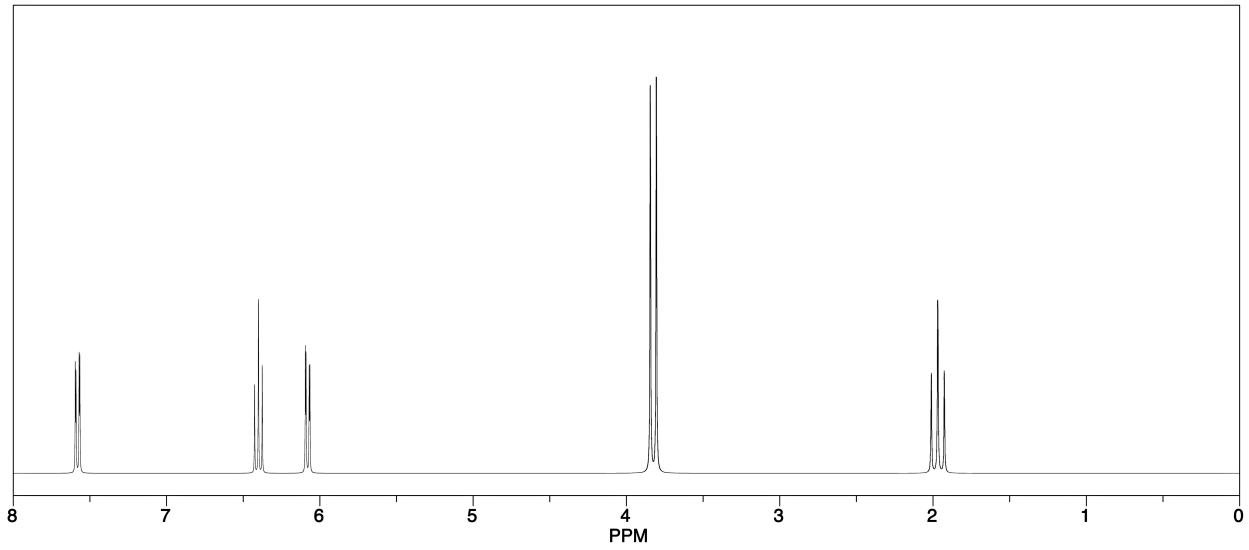
Structure:

Reasoning on how you deduced your structure:

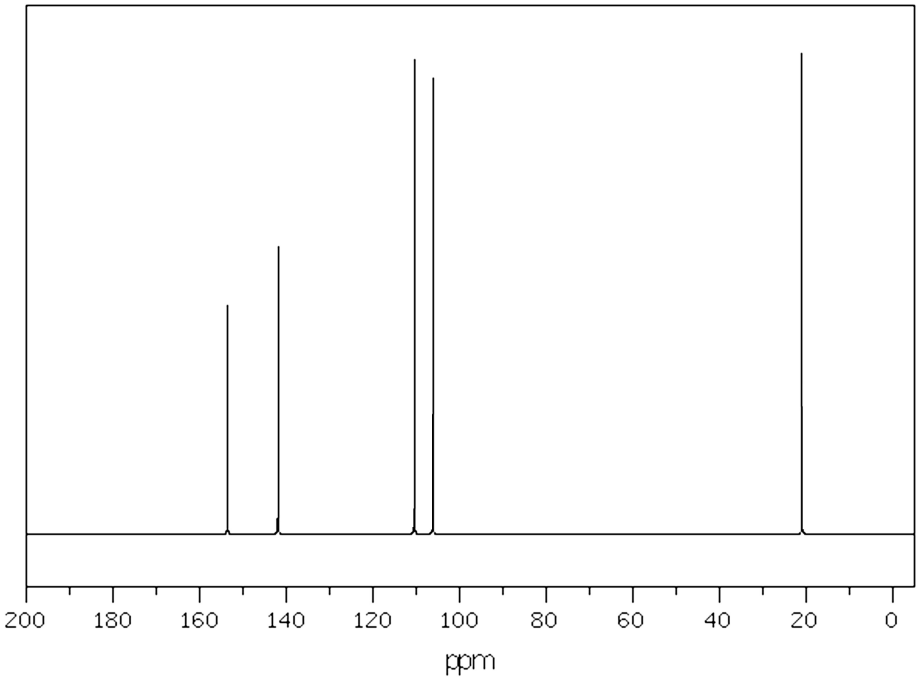
Name

Problem 3 continued…

^{1}H NMR spectrum, with 1:1:1:2:1 integral ratios from left-to-right. Coupling constants for peaks within the same sequence: 7.58 (J = 2.9, 0.9 Hz), 6.40 (J = 3.2, 2.9 Hz), 6.08 (J = 3.2, 0.9 Hz), 3.73 (J = 7.7 Hz), 1.90 (J = 7.7 Hz):



^{13}C NMR spectrum:

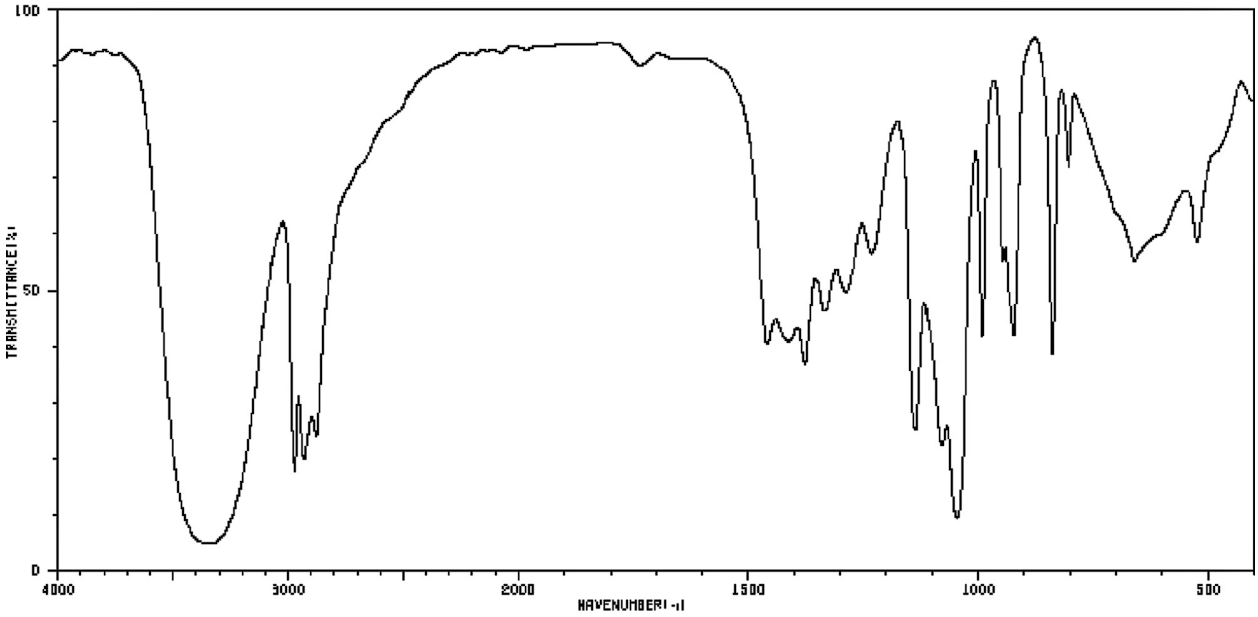


Name

4. (25 points) A compound has the molecular formula $C_6H_{14}O_2$. Deduce its structure from the IR, ^1H NMR and ^{13}C NMR spectra given below:

Degree of unsaturation: _____

IR spectrum (neat film):



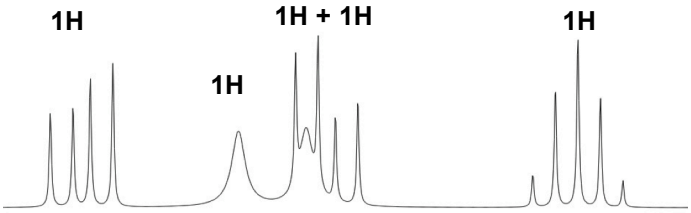
Explain your analysis of the data and deduction of the final structure here:

Name

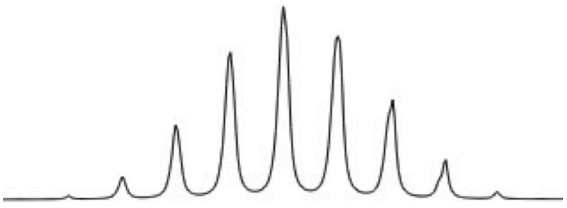
^{1}H NMR spectrum for question 4:

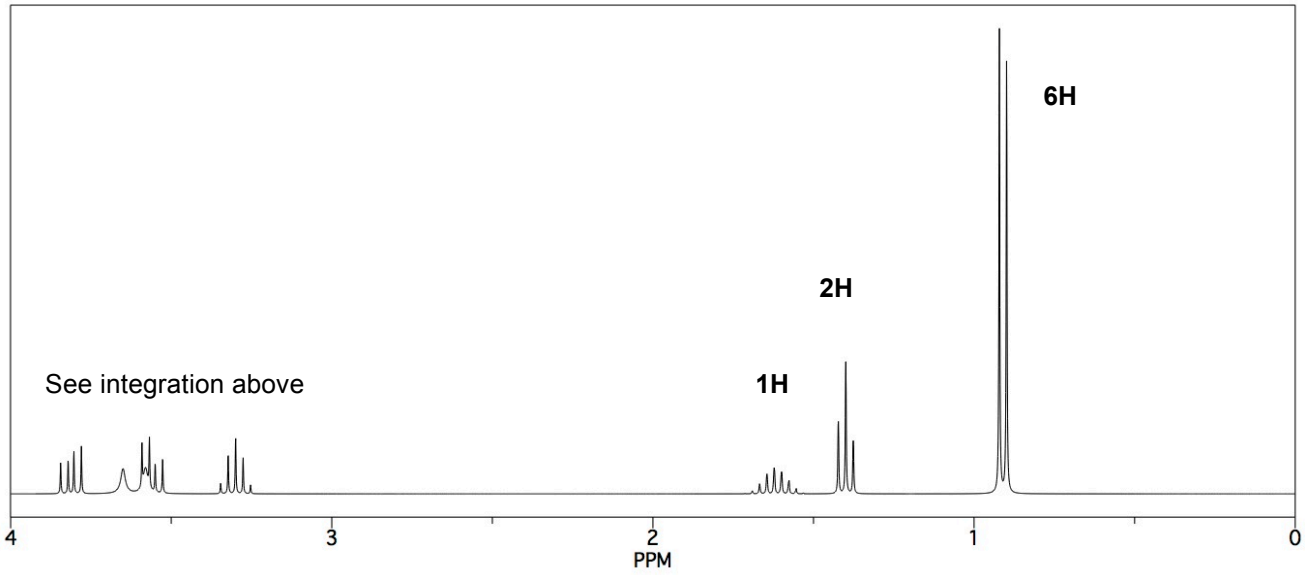
Please draw structure here as well, and provide assignments between protons on structure and relevant peaks using arrows pointing to the peaks in the spectrum:

Expansion of spectrum from 3.2 – 3.9 ppm:



Expansion of spectrum from 1.5 – 1.7 ppm:





Name

^{13}C NMR spectrum for question 4:

Please draw structure here again, and provide assignments for all carbons on the structure and relevant peaks using arrows or letters (note that carbons at 67 and 74 ppm can be assigned based on their degree of substitution).