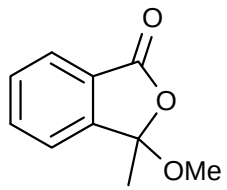
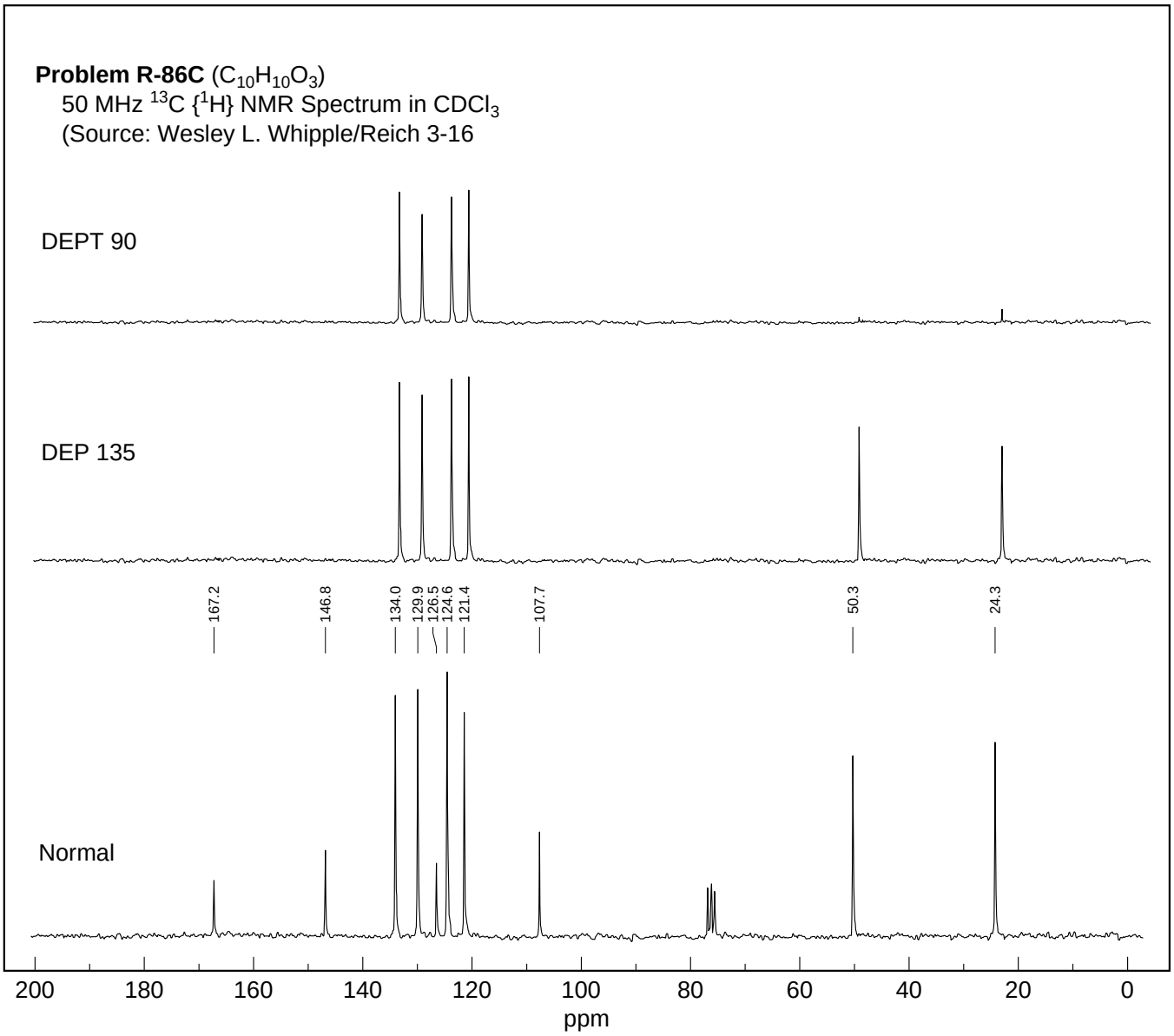
Problem R-86C ($C_{10}H_{10}O_3$)
500.135 MHz ^{1}H NMR Spectrum in $CDCl_3$
(Source: Wesley L. Whipple/Reich (digitized hard copy) 3-16 g



PLT pr-080-to-86.plt

Problem R-86C ($C_{10}H_{10}O_3$)
50 MHz ^{13}C {^1H} NMR Spectrum in $CDCl_3$
(Source: Wesley L. Whipple/Reich 3-16



Problem R-86C ($C_{10}H_{10}O_3$)
IR Spectrum neat
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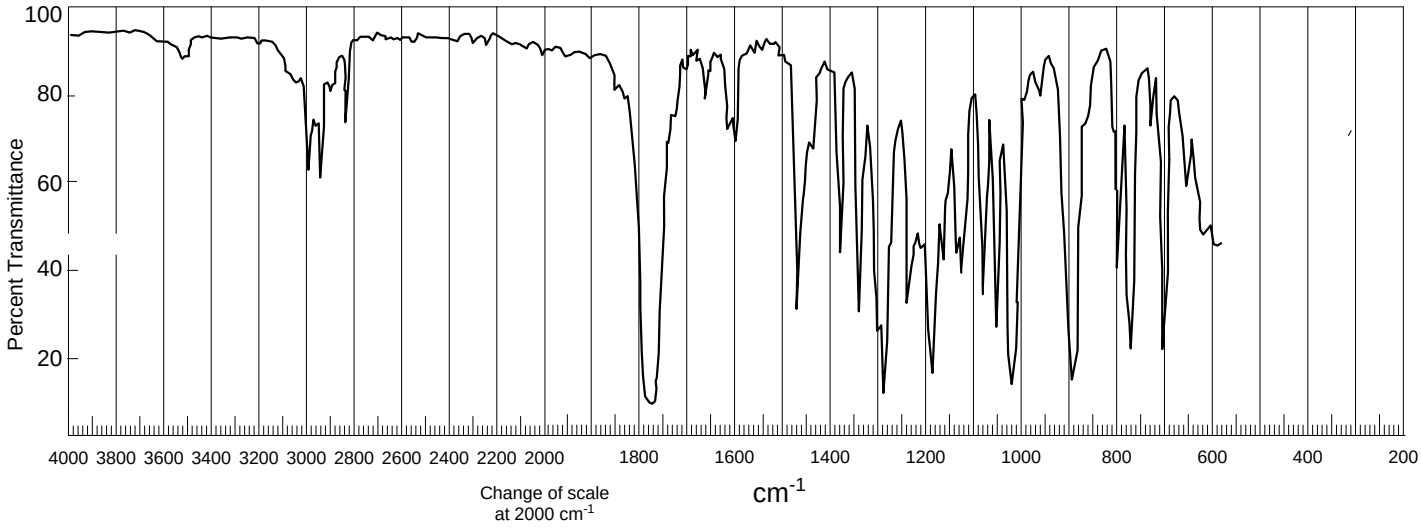

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Problem R-86C ($C_{10}H_{10}O_3$). From the infrared, proton NMR and carbon NMR spectra provided, determine the structure of R-86C. Whether you arrive at a satisfactory answer or not, answer each part below.

(a) DBE _____

(b) Analyze the IR spectrum.

(c) What does the region δ 7 to δ 8 in the ^{1}H NMR spectrum tell you? Draw part structures.

(d) Analyze the ^{13}C NMR spectra. Draw part structures.

(e) Draw possible structures for R-86C below. CIrcle your best guess, and label it with as many of the ^{13}C shifts as you can assign.

Problem R-86C ($C_{10}H_{10}O_3$). From the infrared, proton NMR and carbon NMR spectra provided, determine the structure of R-86C. Whether you arrive at a satisfactory answer or not, answer each part below.

(a) DBE 6

(b) Analyze the IR spectrum.

1780 cm^{-1} ester/lactone, maybe slightly strained ring (5 ring) normal ester at 1740 cm^{-1}

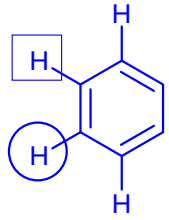
1610 cm^{-1} Aromatic C=C stretch

1200 cm^{-1} Ester C-O stretch

No OH, so the thrteeO must be carbonyl or ether tye

(c) What does the region δ 7 to δ 8 in the ^1H NMR spectrum tell you? Draw part structures.

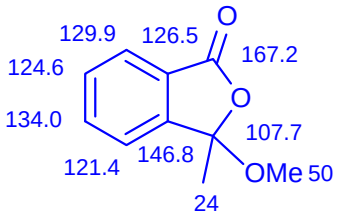
- 4H aromatic region - unsymmetrically disubstituted aromatic ring
- The multiplets at 7.70 and 7.56 (td, J = 8, 1.5 Hz) are each due to a proton with two ortho and one meta coupling



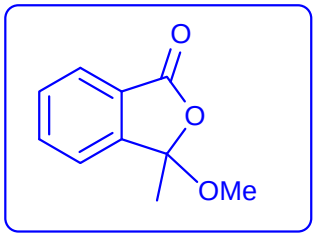
- the dt? are the other two protons, with only one ortho coupling

(d) Analyze the ^{13}C NMR spectra. Draw part structures.

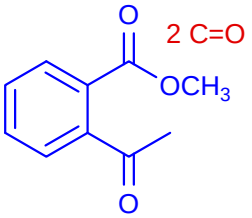
- one OMe at δ 50.3
- one C-CH_3 at δ 24.3 ppm
- one ester/lactone C=O δ 167.2
- one quaternary carbon at δ 107.7 C$(OR)_2$?
- 4 other aromatic C-H carbons

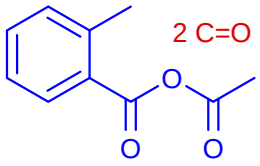


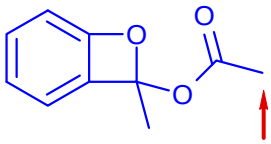
(e) Draw possible structures for R-86C below. CIrcle your best guess, and label it with as many of the ^{13}C shifts as you can assign.



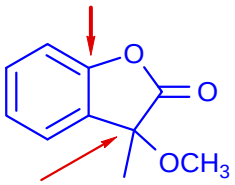
expect ca δ 160 not 147



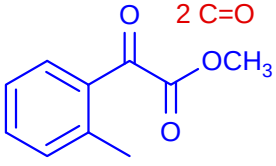


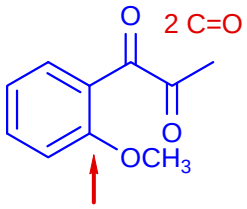


expect δ 25, not 50

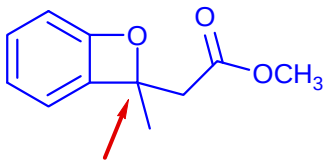


Expect 80?





expect ca δ 160 not 147



expect 70, not 108

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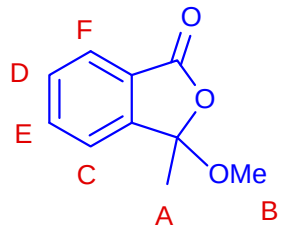

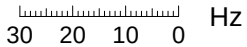

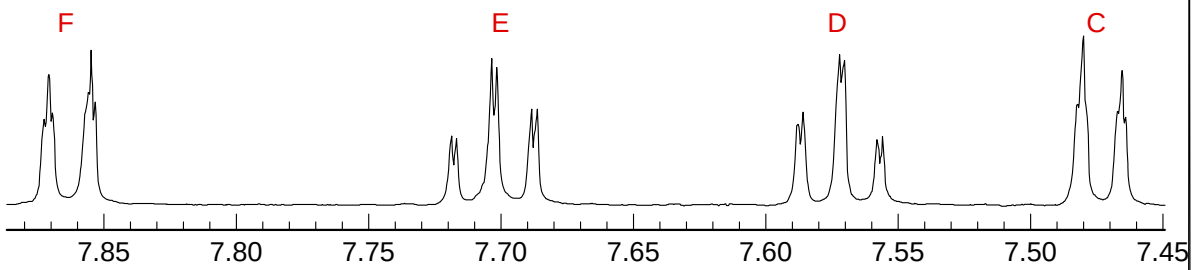

Somewhat unusual O-CH_3 - presumaably the CH_3 is in the shielding region of the benzene ring

A little too far upfield for CH_3-C=O

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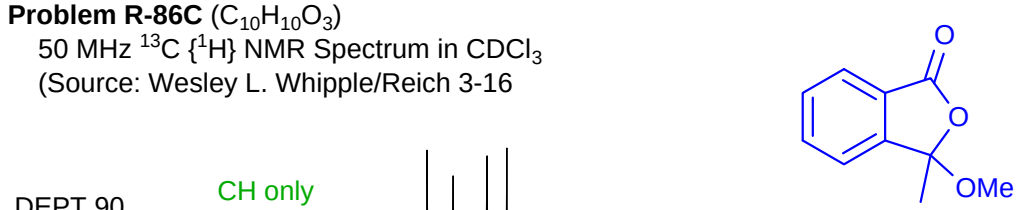

Problem R-86C ($C_{10}H_{10}O_3$)
IR Spectrum neat
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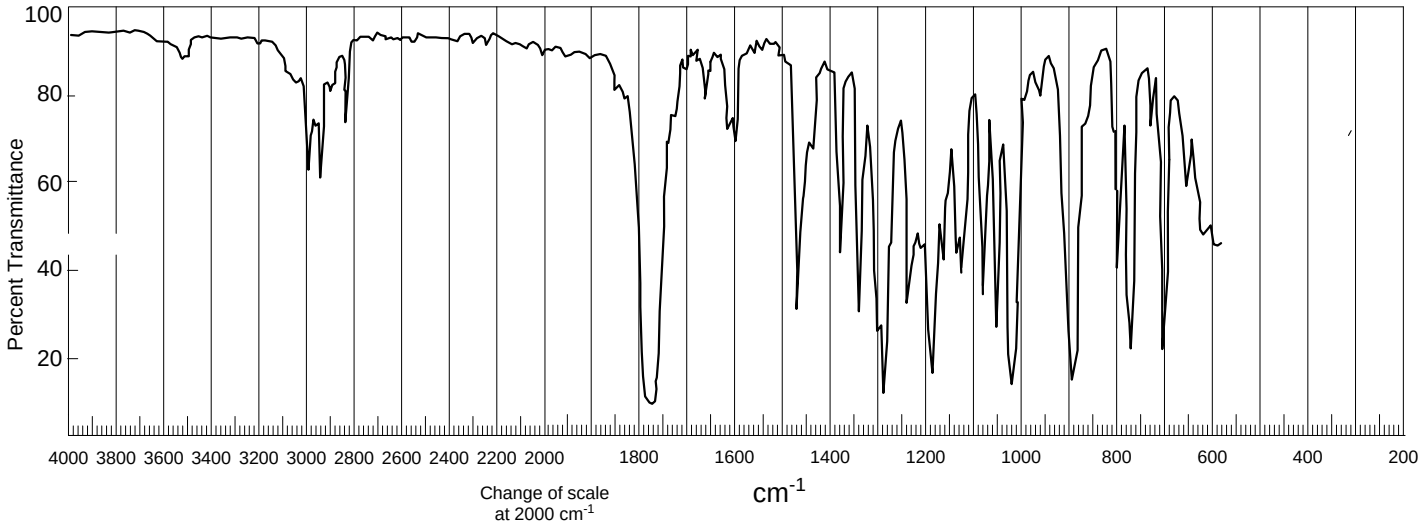

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