Problem R-07F ($C_8H_{14}O_4$)

300 MHz ^1H NMR spectrum

Source: Aldrich Spectra Collection/Reich g
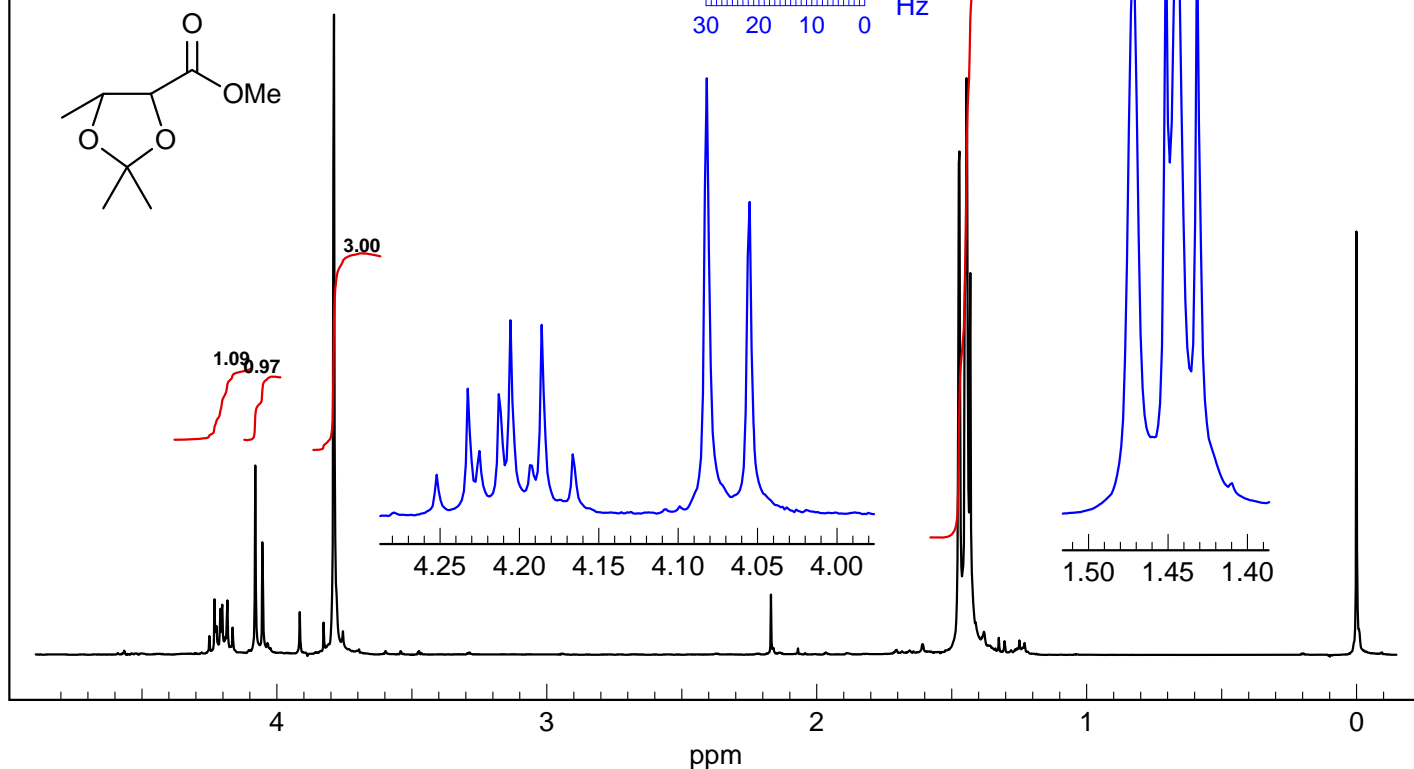
9.28

3.00

1.09 0.97

Hz

30 20 10 0

4.25 4.20 4.15 4.10 4.05 4.00

1.50 1.45 1.40

ppm

4 3 2 1 0

Problem R-07F ($C_8H_{14}O_4$)

75 MHz ^{13}C NMR spectrum

Source: Aldrich Spectra Collection

DEPT 90

DEPT 135

170.8

110.4

80.3

75.0

52.1

27.1
25.6

18.5

Normal

200 180 160 140 120 100 80 60 40 20 0

ppm

PLT ex-1-2007-08-gq.plt
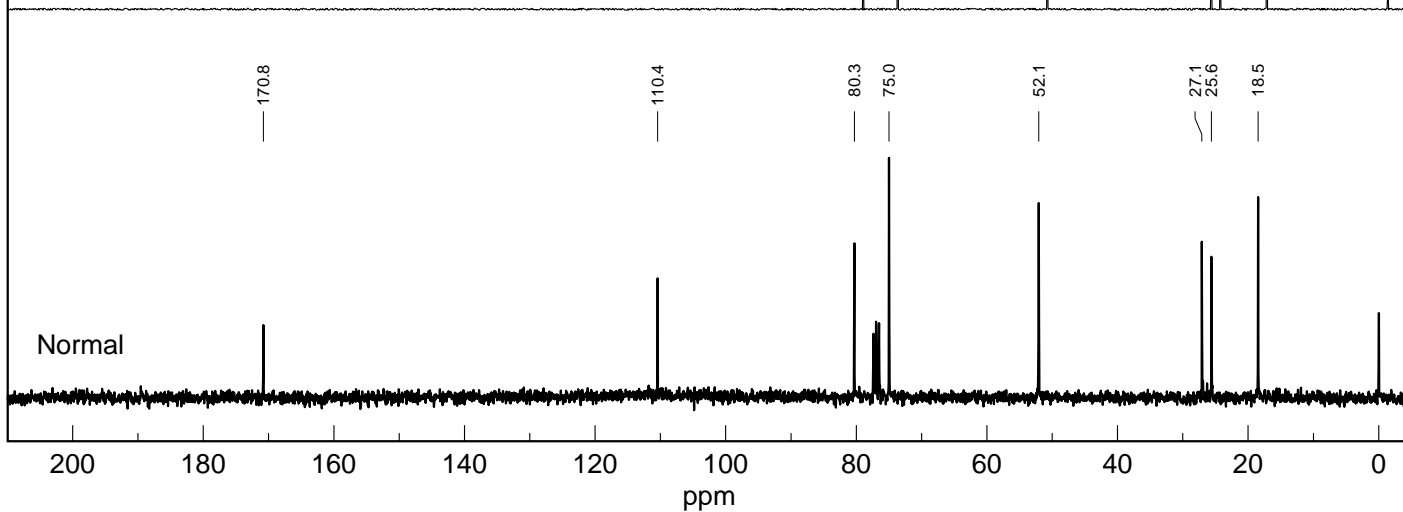
Problem R-07F ($C_8H_{14}O_4$). Determine the structure of the compound from the ^1H and ^{13}C NMR spectra given.
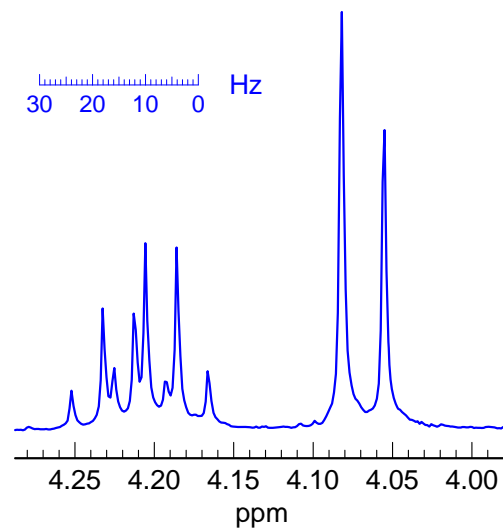
(a) DBE_____

(b) The IR spectrum shows a strong signal at 1735 cm^{-1}. What does this tell you?

(c) Interpret the ^{13}C NMR spectrum. Use the Normal, DEPT-135 and DEPT 90 spectra to help in the analysis. Identify what kind of carbon each signal corresponds to and write possible part structures (you may wish to examine all the data before completing this section).

Type of C (e.g. sp^3 CH$_2$) and/or part structures (e.g. N-CH$_2$)

18.5	_____	75.0	_____
25.6	_____	80.3	_____
27.1	_____	110.4	_____
52.1	_____	170.8	_____

(d) Interpret the ^1H signals between δ 4.0 and 4.4. Give part structures, shifts, and any couplings

(d)   Draw the structure of **R-07F**. If more than one structure is possible, show them, and circle the one you think fits the data best and give your reasons for choosing it.

Problem R-07F ($C_8H_{14}O_4$). Determine the structure of the compound from the ^1H and ^{13}C NMR spectra given.

2

(a) DBE __2__

(b) The IR spectrum shows a strong signal at 1735 cm^{-1}. What does this tell you?

2

There is a carbonyl in the molecule, probably an ester or lactone

(c) Interpret the ^{13}C NMR spectrum. Use the Normal, DEPT-135 and DEPT 90 spectra to help in the analysis. Identify what kind of carbon each signal corresponds to and write possible part structures (you may wish to examine all the data before completing this section).

Type of C (e.g. sp^3 CH$_2$) and/or part structures (e.g. N-CH$_2$)

7

18.5	CH$_3$-C	75.0	sp^3 H-C-O
25.6	CH$_3$-C	80.3	sp^3 H-C-O
27.1	CH$_3$-C	110.4	sp^3 C(OR)$_2$, possible -C≡C-
52.1	CH$_3$O	170.8	sp^2 O=C-OR, ester carbonyl

(d) Interpret the ^1H signals between δ 4.0 and 4.4. Give part structures, shifts, and any couplings

6

4.07
d, J= 8

4.20
dq, J = 8, 6

Possibly:

dq, J = 8, 6
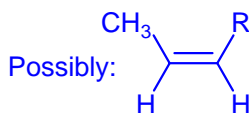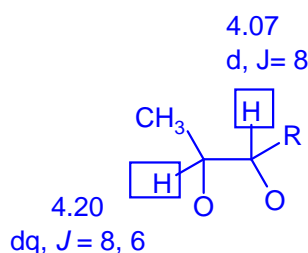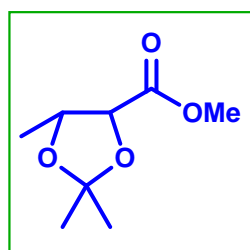
The chemical shift requires α-oxygen substitutents Or possibly vinyl protons), the couplings shows an isolated CH$_3$-CH-CH spin system
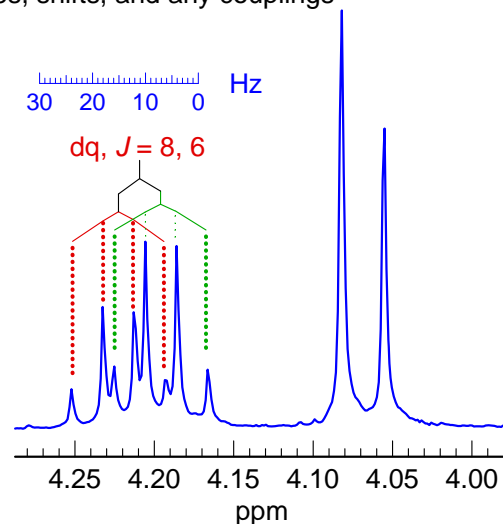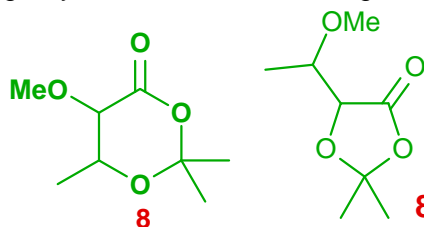

(d) Draw the structure of **R-07F**. If more than one structure is possible, show them, and circle the one you think fits the data best and give your reasons for choosing it.
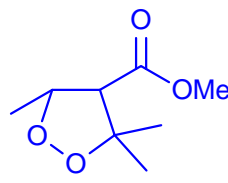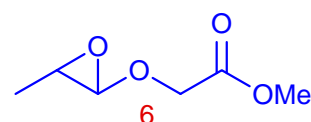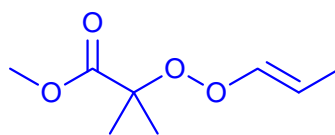
8

8

8

8

7

6

These two also fit the NMR data

6

5

5

Problem R-07F (C₈H₁₄O₄)

Problem R-07F ($C_8H_{14}O_4$)

300 MHz ^{1}H NMR spectrum

Source: Aldrich Spectra Collection

30 20 10 0 Hz

8.49

2.74

1.00 0.88

4.25 4.20 4.15 4.10 4.05 4.00

1.50 1.45 1.40

ppm

Problem R-07F ($C_8H_{14}O_4$)

75 MHz ^{13}C NMR spectrum

Source: Aldrich Spectra Collection

DEPT 90

DEPT 135

170.8

110.4

80.3 75.0

52.1

27.1 25.6

18.5

O

O   O

H-C-O

H-C-O

CH₃-O

CH₃-C

O

OMe

Normal

200 180 160 140 120 100 80 60 40 20 0

ppm

PLT ex-1-2007-08-gq.plt