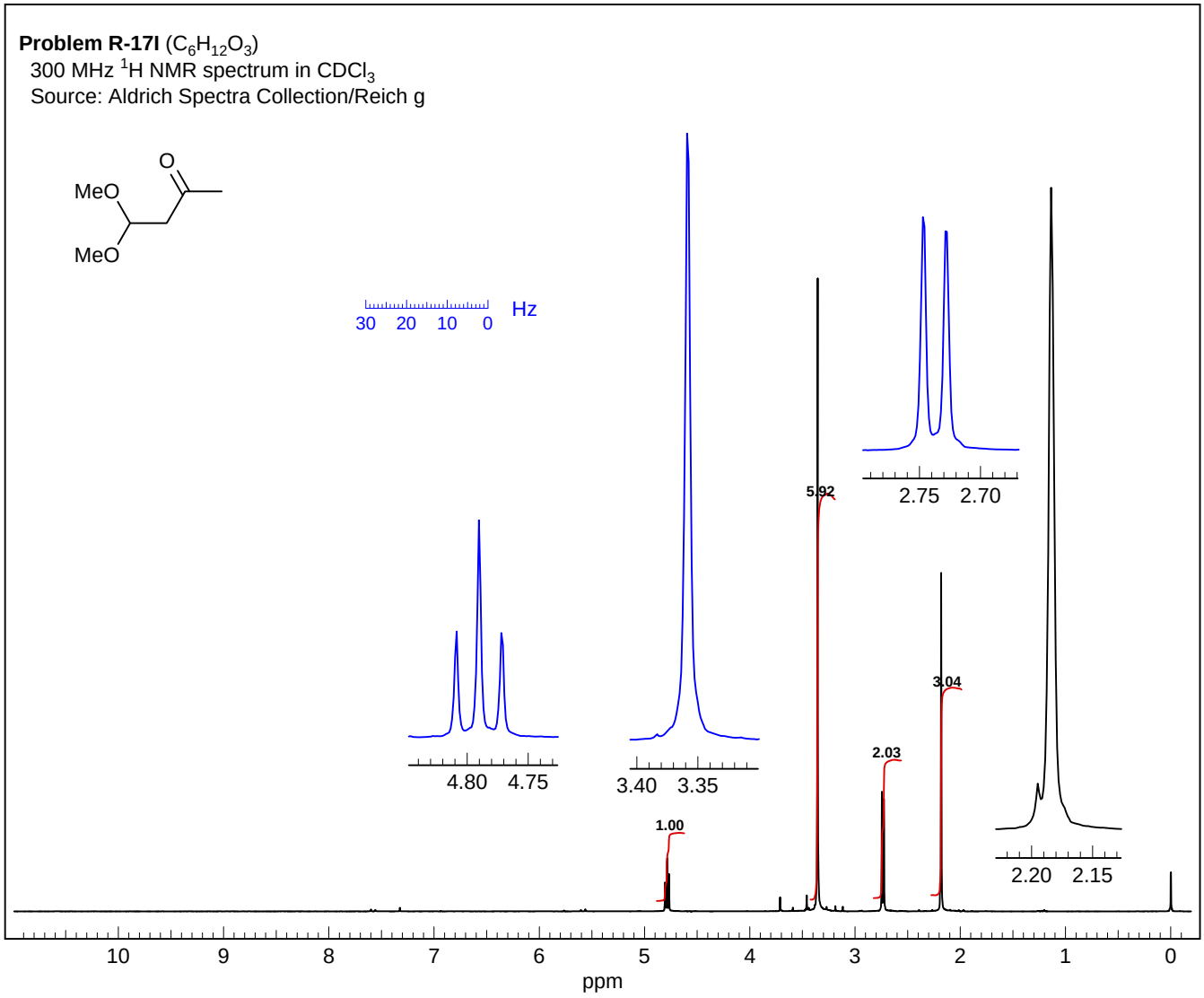
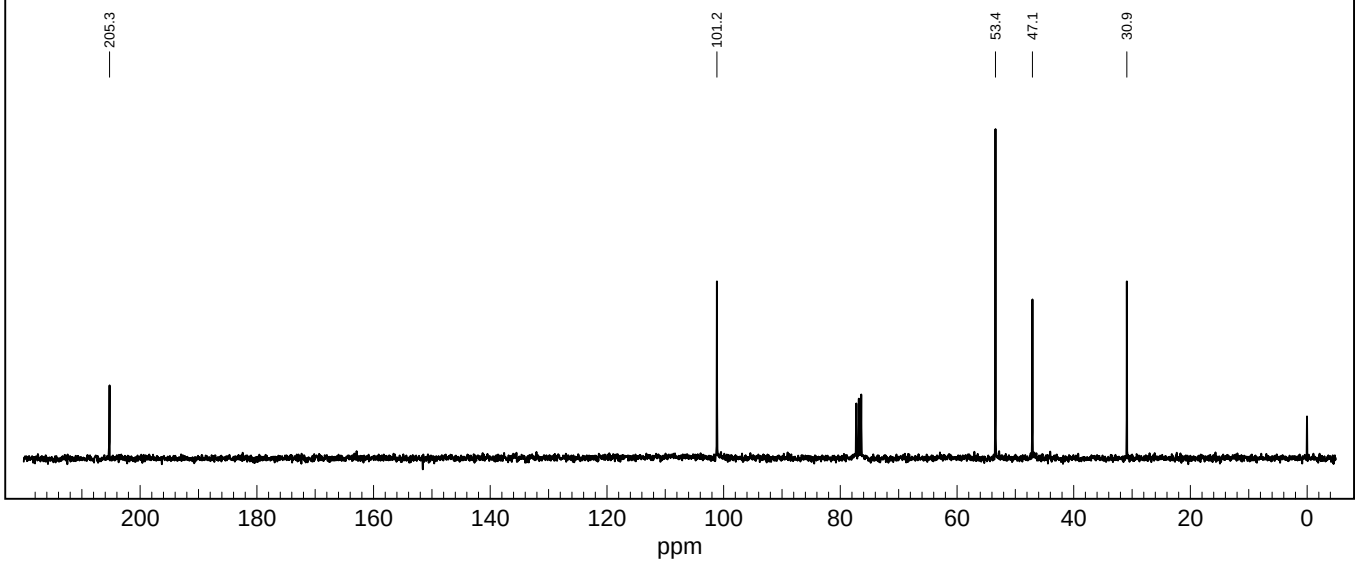
Problem R-17l ($C_6H_{12}O_3$)
300 MHz ^{1}H NMR spectrum in $CDCl_3$
Source: Aldrich Spectra Collection/Reich g



Problem R-17l: $C_6H_{12}O_3$
75 MHz ^{13}C NMR spectrum in $CDCl_3$
Source: Aldrich Spectral Viewer/Reich



PLT pr-017-proton-carbon-x.plt

Chem 345-2
Reich Exam 1
October 5, 2009

1. (15.) Determine the structure of $C_6H_{12}O_3$ from the ^1H NMR spectrum shown. Write part structures revealed by the chemical shifts, splitting and integrals for all the multiplets. In each part structure **circle** the hydrogens responsible for the absorption and **underline** the hydrogens that give rise to the splitting. Even if your structure is correct, you will not get full credit without writing the part structures.

Number of unsaturations = _____

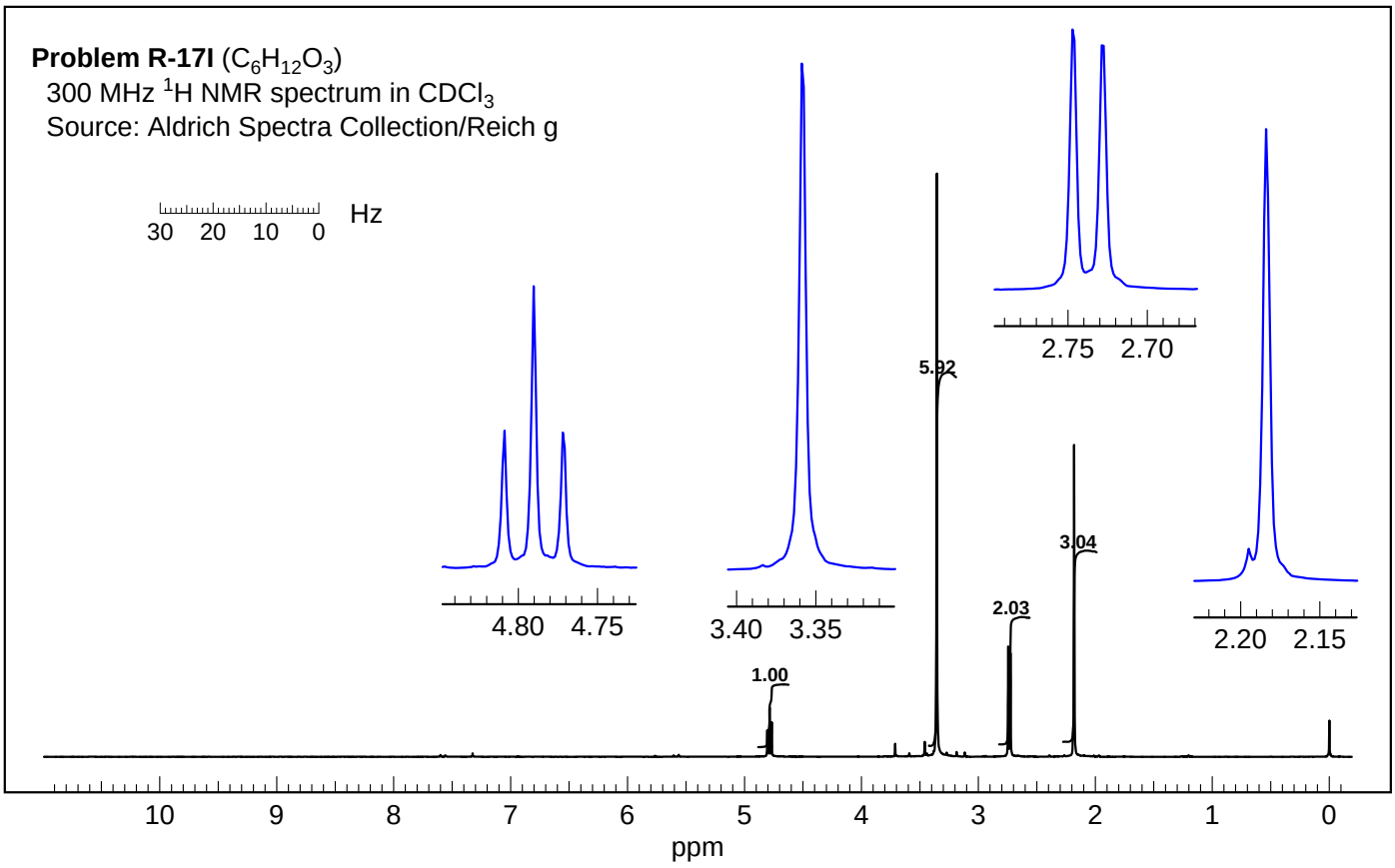
Part structures at δ **2.2**

2.7

3.4

4.8

Complete Structure:



PLT pr-017-proton-carbon-x.plt

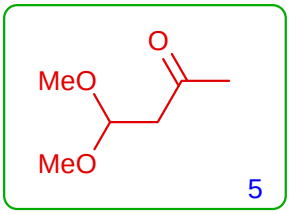
1. (15.) Determine the structure of $C_6H_{12}O_3$ from the ^1H NMR spectrum shown. Write part structures revealed by the chemical shifts, splitting and integrals for all the multiplets. In each part structure **circle** the hydrogens responsible for the absorption and **underline** the hydrogens that give rise to the splitting. Even if your structure is correct, you will not get full credit without writing the part structures.

Number of unsaturations = 1

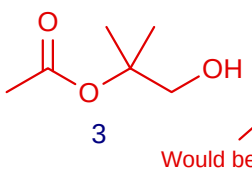
Part structures at δ

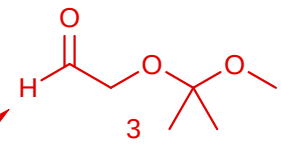
2.2	-CH_3	2
2.7	CH–CH_2	2
3.4	2x -O-CH_3	2
4.8	CH–CH_2	2

Complete Structure:

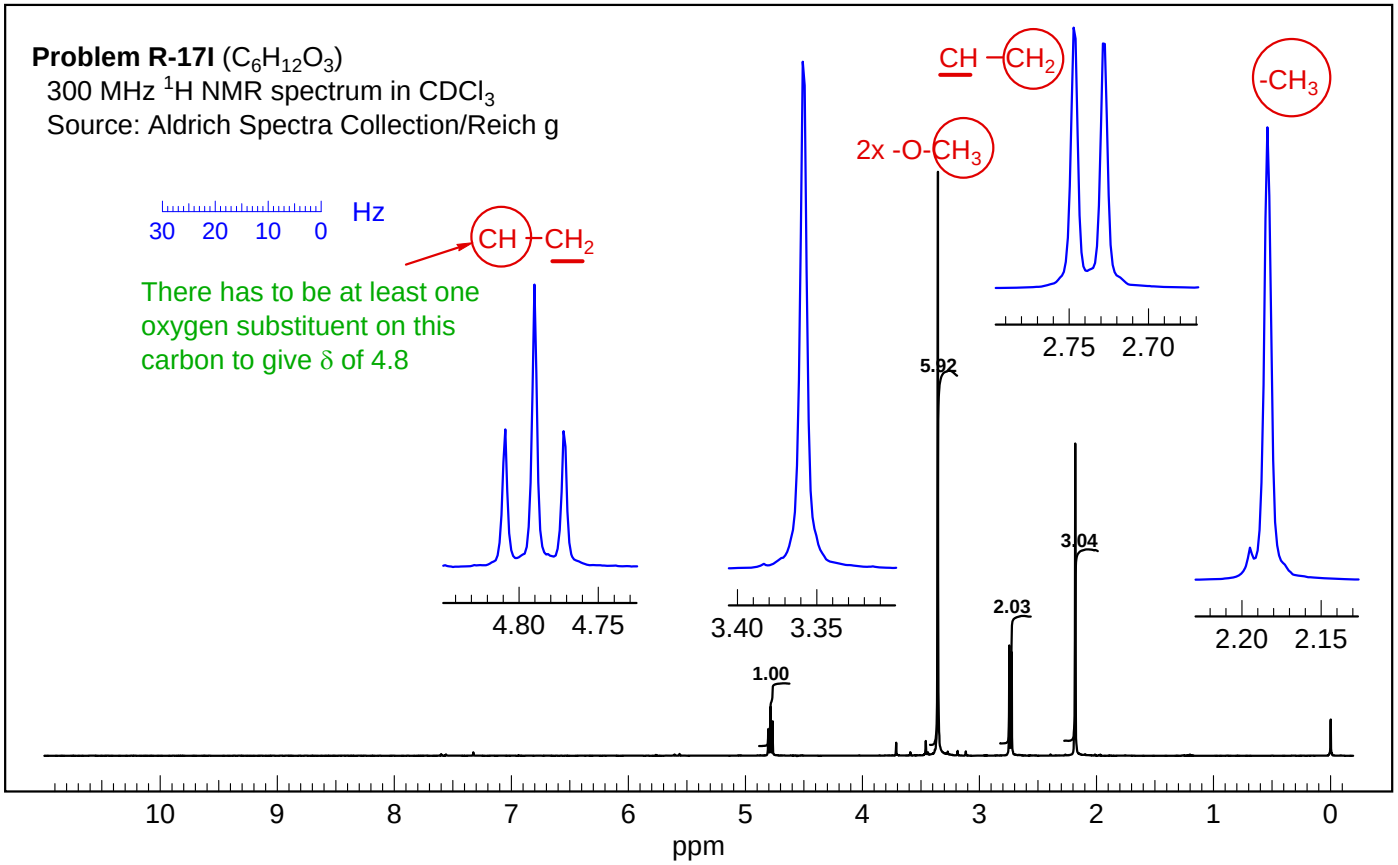


These sort of fit the NMR spectrum

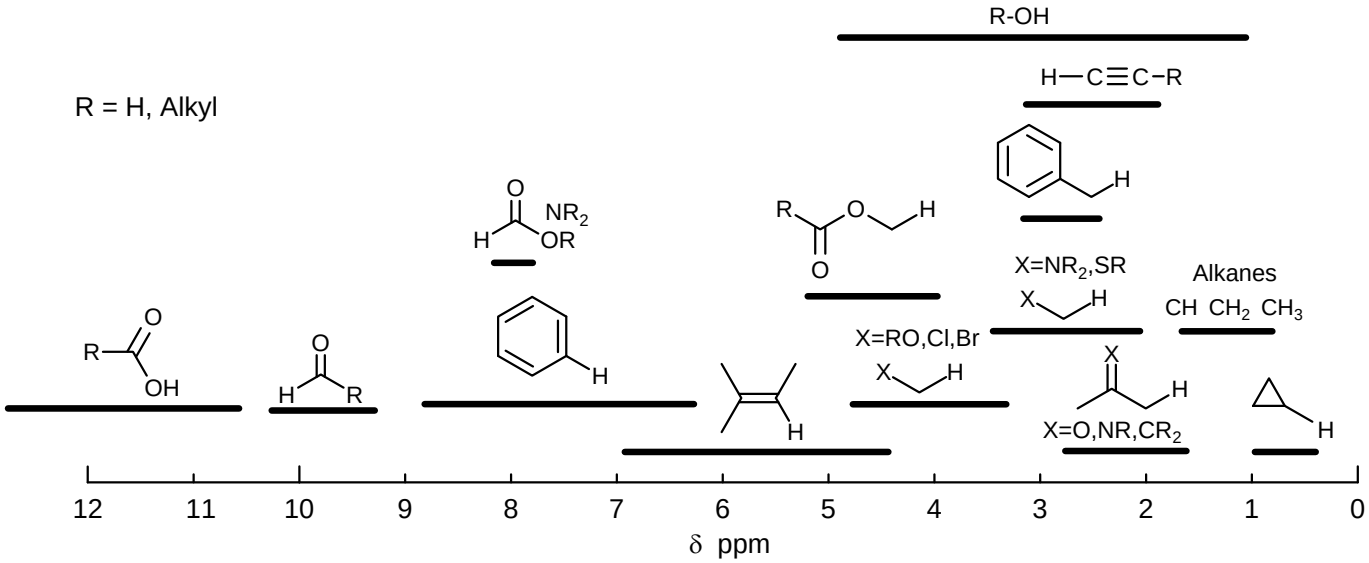




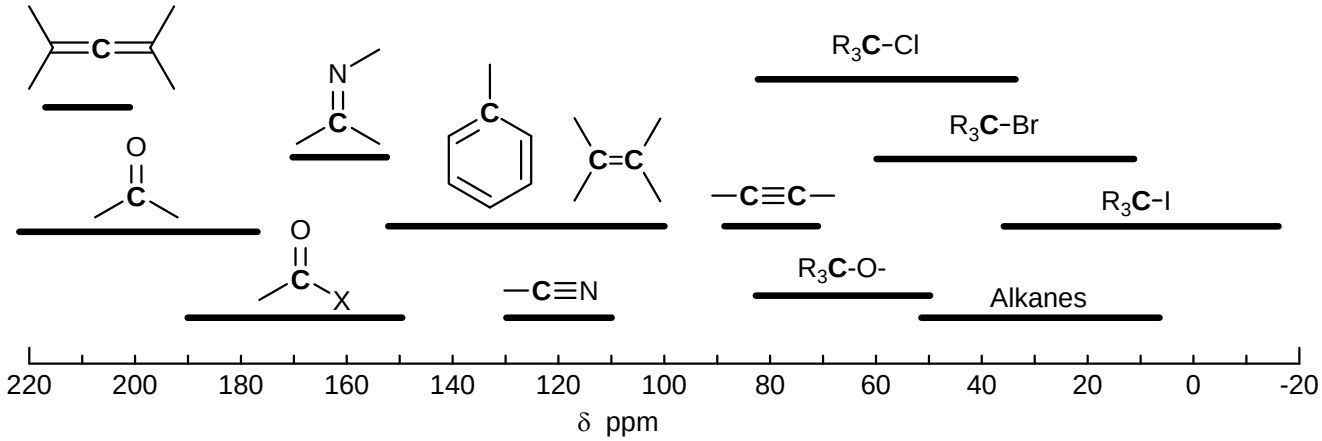
Would be at δ 10



Proton Chemical Shifts



Carbon-13 Chemical Shifts



Principal Infrared Absorptions

C-H Stretching vibrations

3630-3200 cm^{-1}	OH
3500-3200	NH
3300-3200	H−C≡C-R (sharp)
3080-3000	CH of alkene, aromatic
2600-2550	SH

Triple Bond Stretch

2250 cm^{-1}	R−C≡N
2225	C=C−C≡N (conjugated)
2150-2100	R−C≡C−R' (weak)

Other Vibrations

1200-1050 cm^{-1}	C-O Single bond stretch

Double Bond Stretching Vibrations

1710 cm^{-1}	Aldehyde or ketone
1680	Conjugated ketone
1745	Cyclopentanone
1780	Cyclobutanone
1730	α-Hydroxy ketone
1740	Ester
1660	Amide
1800	Acid chloride
1810 and 1760	Acid anhydride
1700	Carboxylic acid
1680-1500	C=C stretch
1675-1590	Aromatic C=C stretch