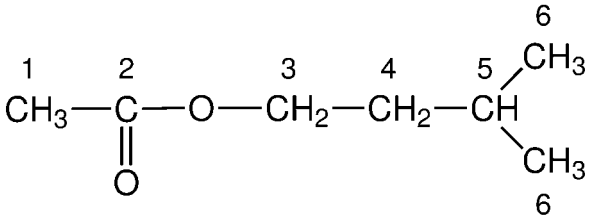
Problem 9

The ^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of isoamyl acetate ($C_7H_{14}O_2$) recorded in $CDCl_3$ solution at 298 K and 600 MHz are given below.

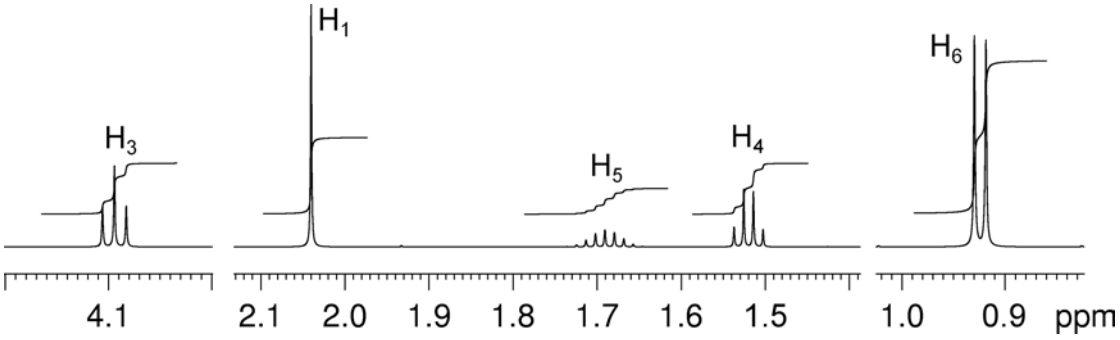
The ^{1}H NMR spectrum has signals at δ 0.92 (H_6), 1.52 (H_4), 1.69 (H_5), 2.04 (H_1) and 4.09 (H_3) ppm.

The $^{13}C\{^{1}H\}$ NMR spectrum has signals at δ 21.0 (C_1), 22.5 (C_6), 25.1 (C_5), 37.4 (C_4), 63.1 (C_3) and 171.2 (C_2) ppm.

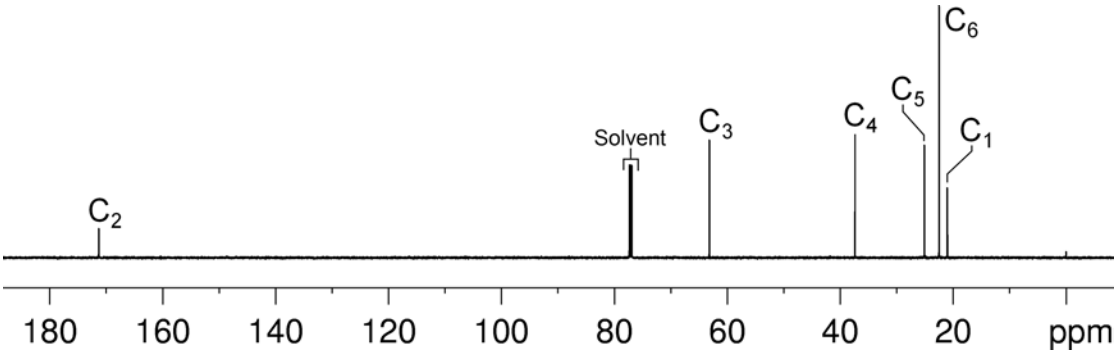
Also given on the following pages are the ^{1}H–^{1}H COSY, ^{1}H–^{13}C me-HSQC, ^{1}H–^{13}C HMBC and INADEQUATE spectra. For each 2D spectrum, indicate which correlation gives rise to each cross-peak by placing an appropriate label in the box provided.

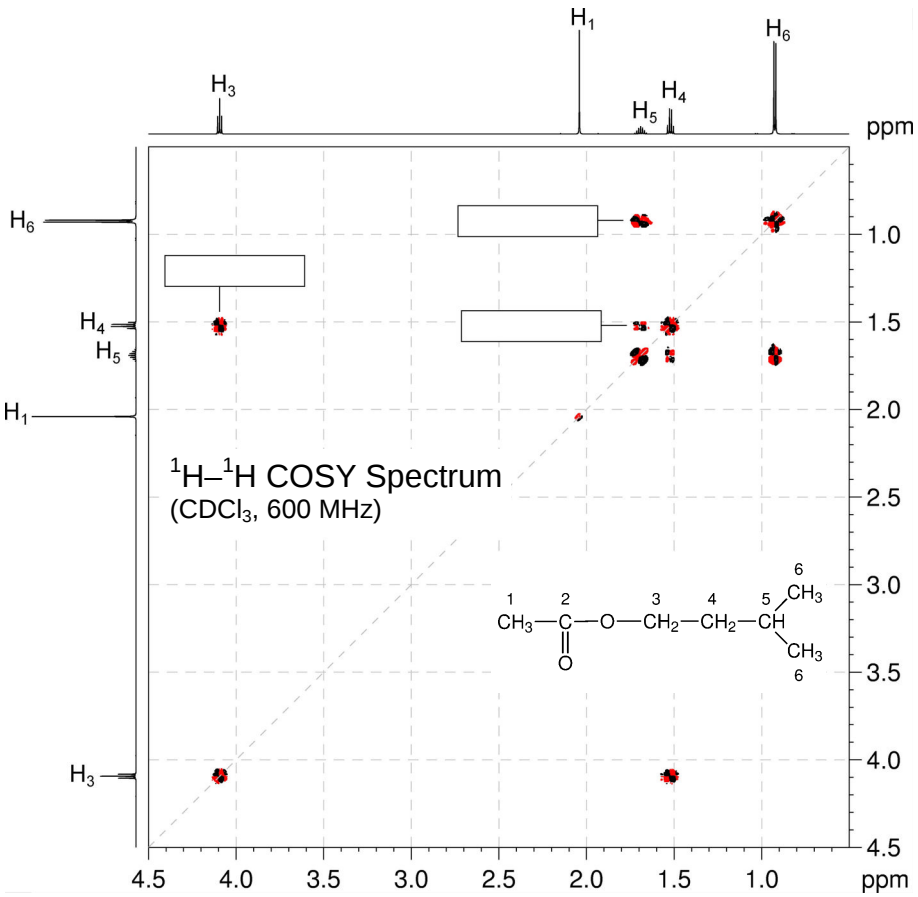


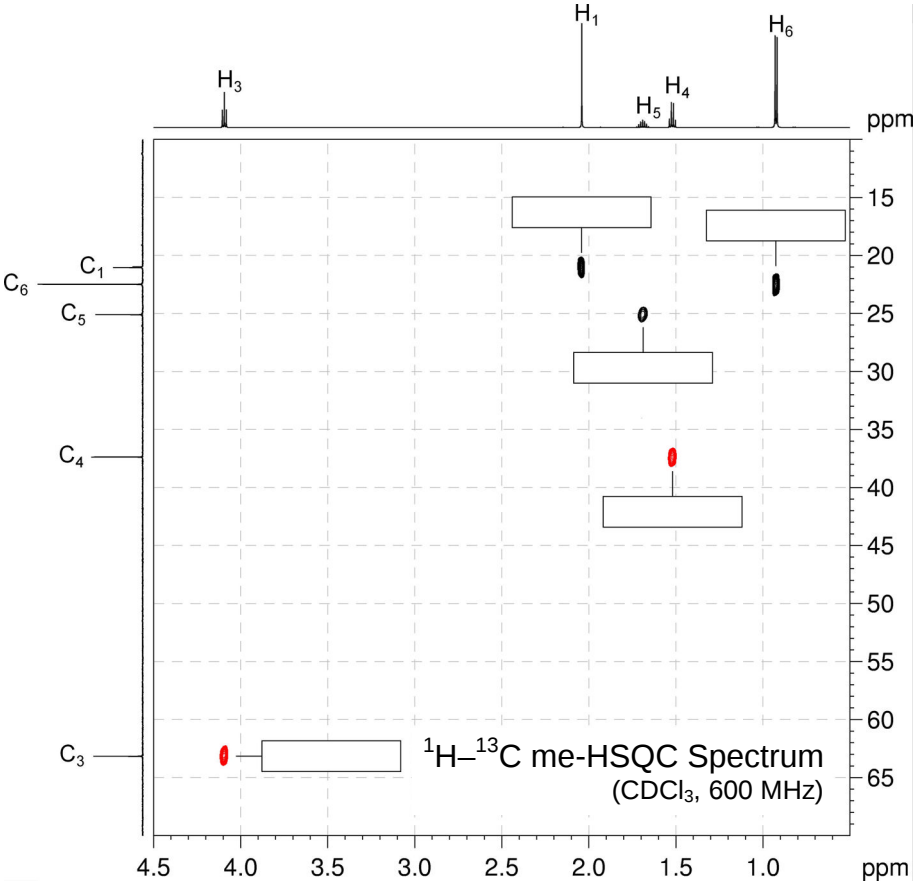
^{1}H NMR Spectrum
($CDCl_3$, 600 MHz)

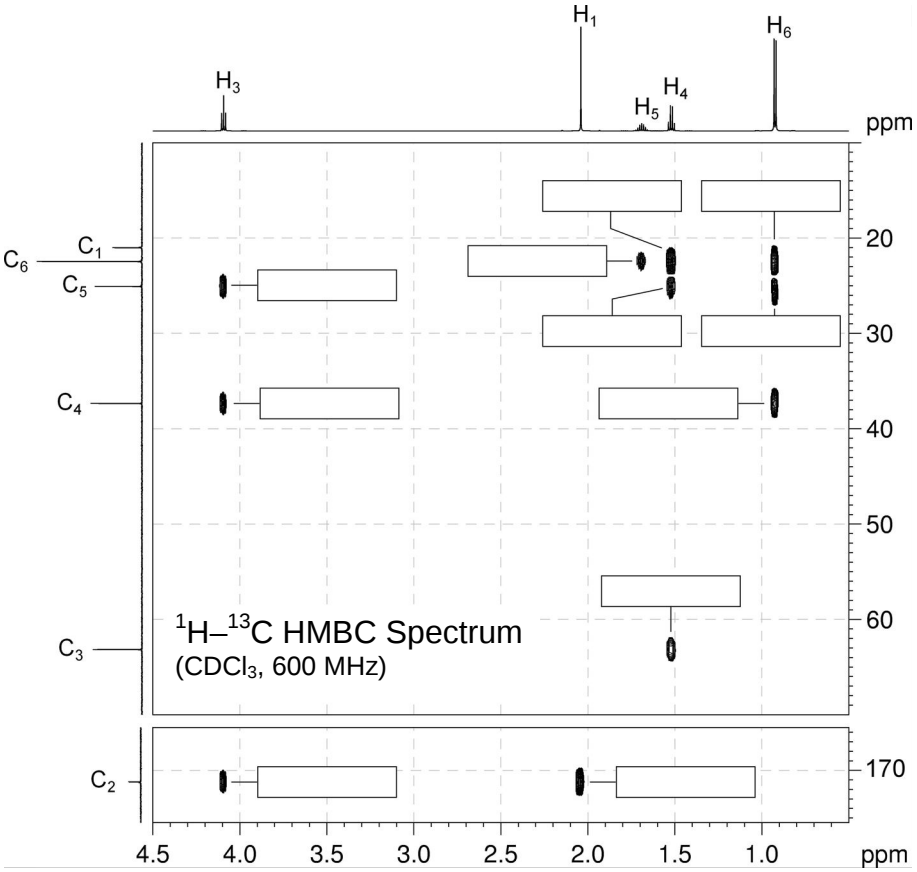


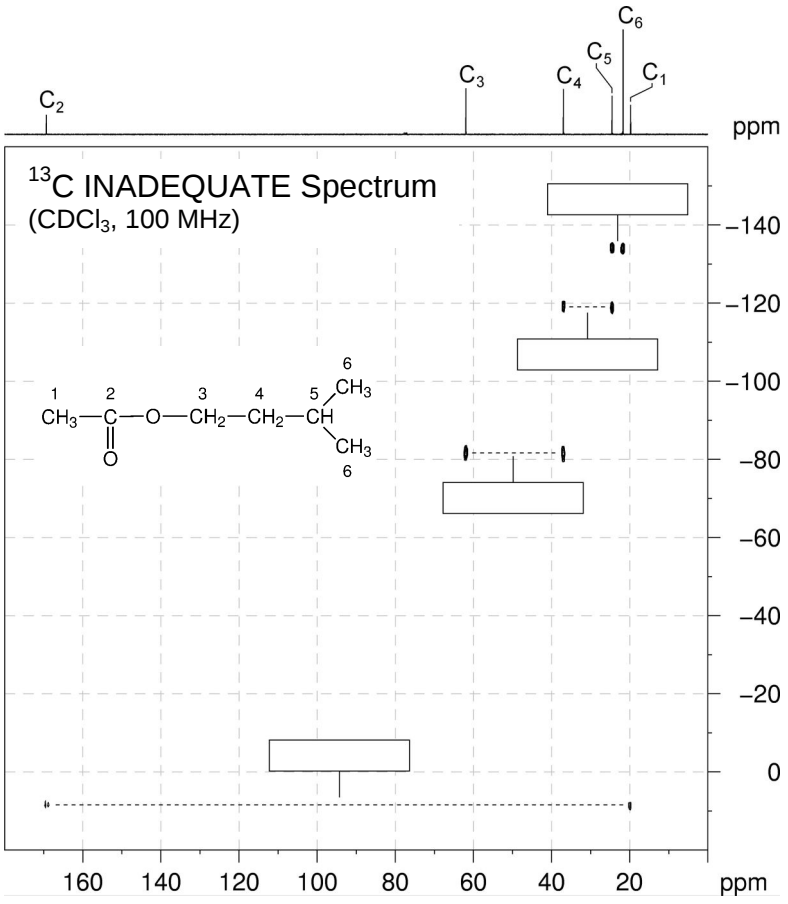
$^{13}C\{^{1}H\}$ NMR Spectrum
($CDCl_3$, 150 MHz)




H1
H6
H3
H4
H5
ppm
H6
H4
H5
H1
H3
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
1H–1H COSY Spectrum
(CDCl3, 600 MHz)
1 2 3 4 5 6
CH3—C—O—CH2—CH2—CH(CH3)
O
4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm


H1
H6
H3
H4
H5
ppm
C1
C6
C5
C4
C3
15
20
25
30
35
40
45
50
55
60
65
1H–13C me-HSQC Spectrum
(CDCl3, 600 MHz)
4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm


H1
H6
H3
H4
H5
ppm
C1
C6
C5
C4
C3
C2
20
30
40
50
60
170
1H–13C HMBC Spectrum
(CDCl3, 600 MHz)
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm


C6
C5
C3
C4
C1
C2
ppm
13C INADEQUATE Spectrum
(CDCl3, 100 MHz)
–140
–120
–100
–80
–60
–40
–20
0
160
140
120
100
80
60
40
20
ppm