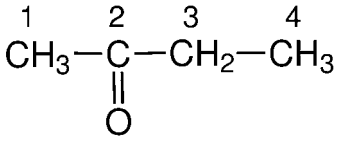
Problem 2

The ^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of 2-butanone (C_4H_8O) recorded in $CDCl_3$ solution at 298 K and 400 MHz are given below.

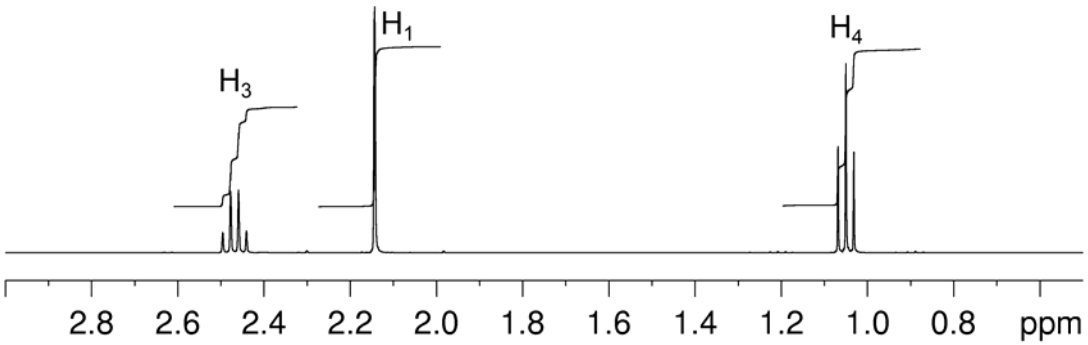
The ^{1}H NMR spectrum has signals at δ 1.05 (H_4), 2.14 (H_1) and 2.47 (H_3) ppm.

The $^{13}C\{^{1}H\}$ NMR spectrum has signals at δ 7.2 (C_4), 28.8 (C_1), 36.2 (C_3) and 208.8 (C_2) ppm.

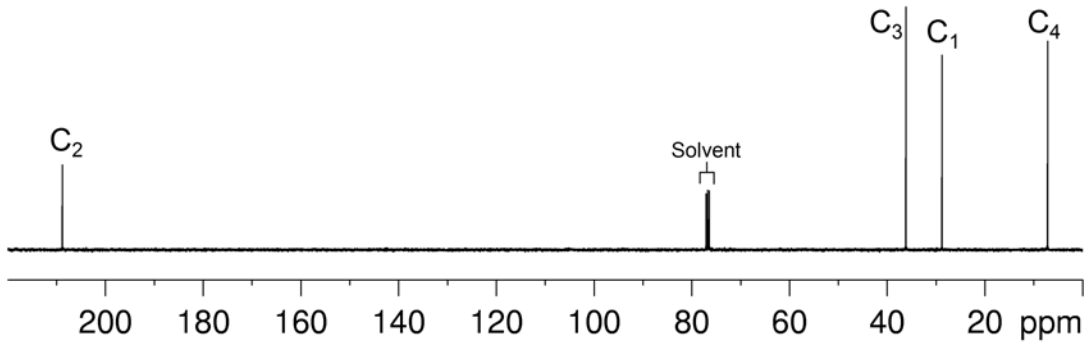
Also given on the following pages are the ^{1}H–^{1}H COSY, ^{1}H–^{13}C me-HSQC, ^{1}H–^{13}C HMBC and INADEQUATE spectra. For each 2D spectrum, indicate which correlation gives rise to each cross-peak by placing an appropriate label in the box provided (*e.g.* $H_1 \rightarrow H_2$, $H_1 \rightarrow C_1$).

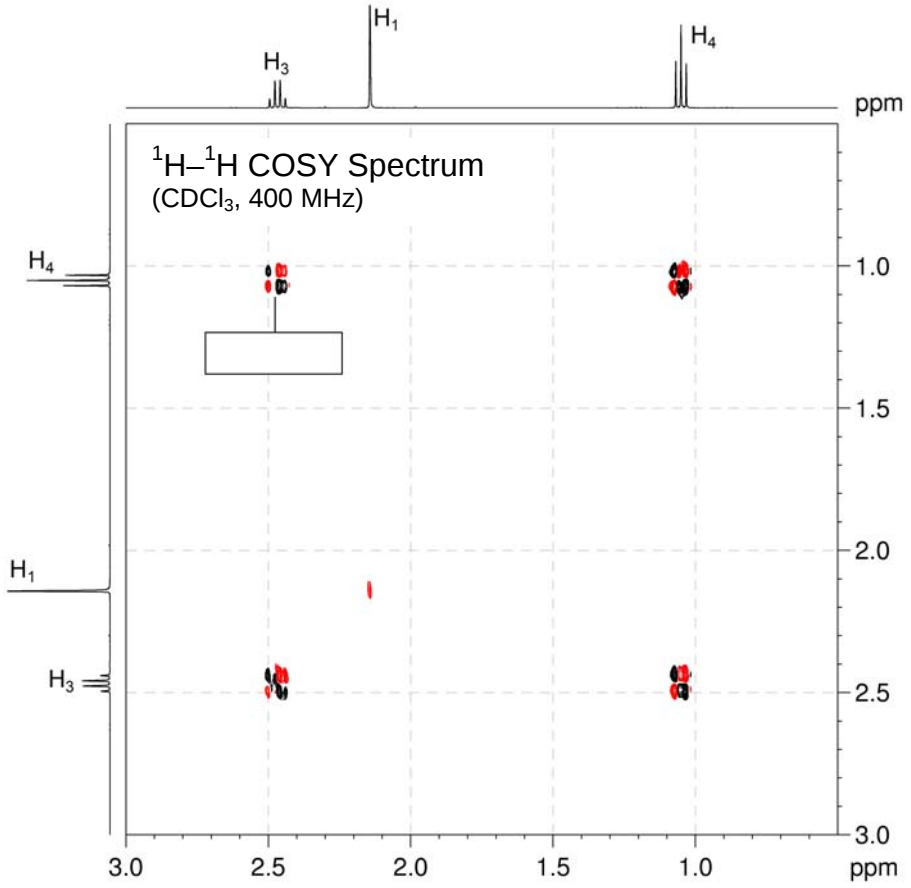


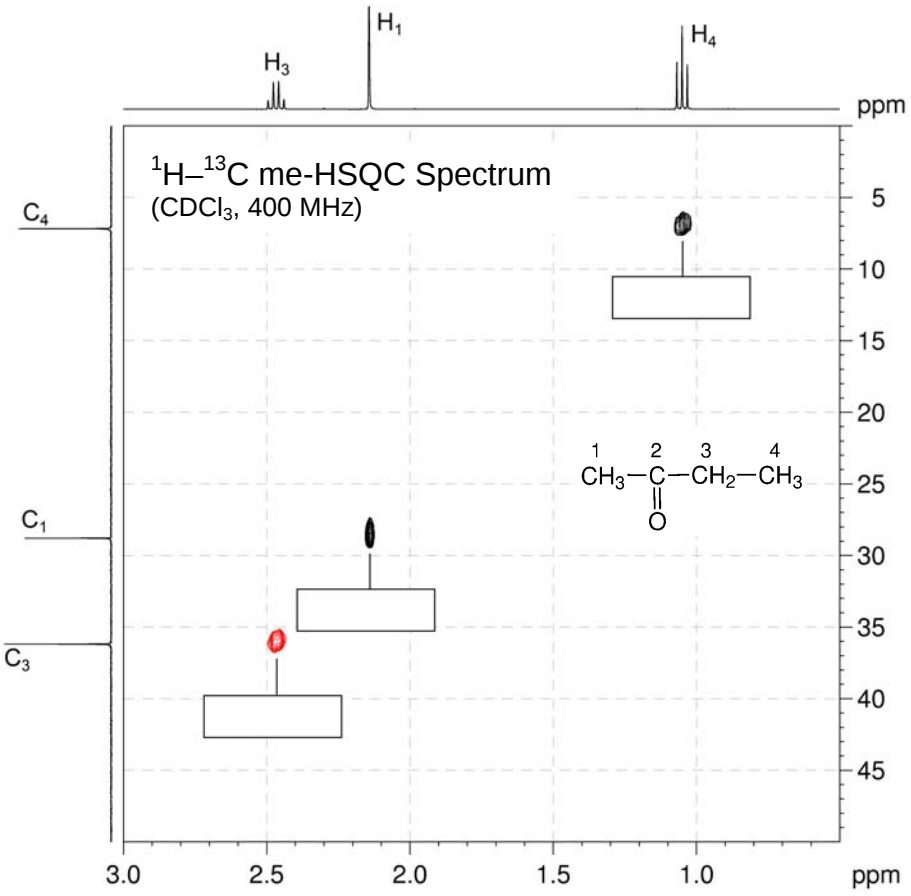
^{1}H NMR Spectrum
($CDCl_3$, 400 MHz)

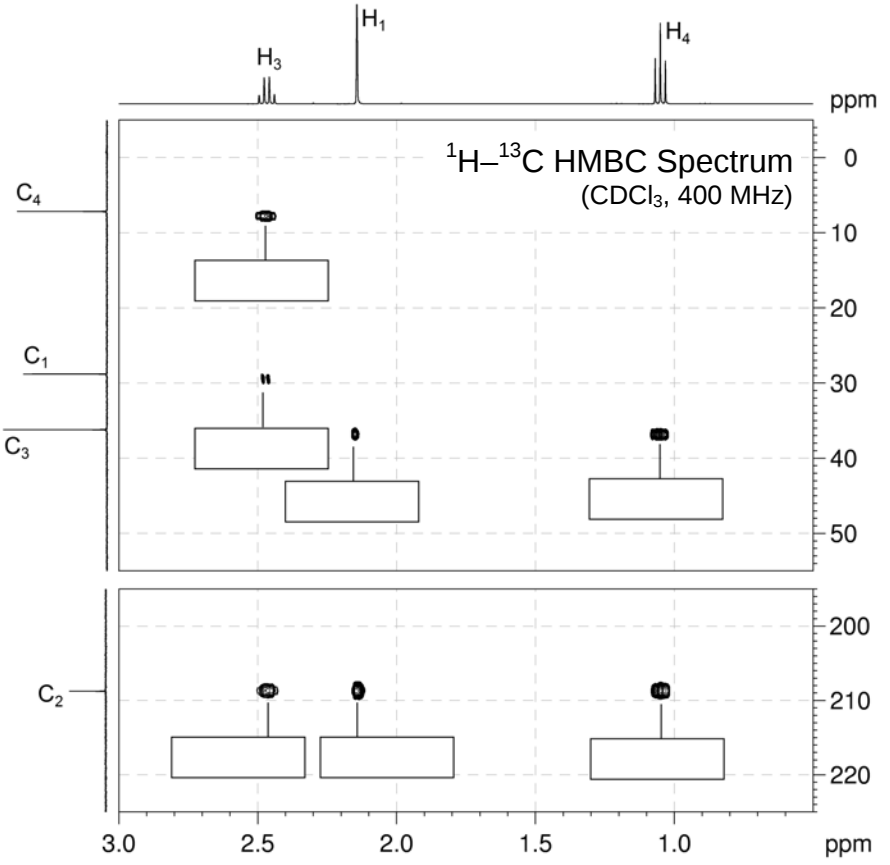


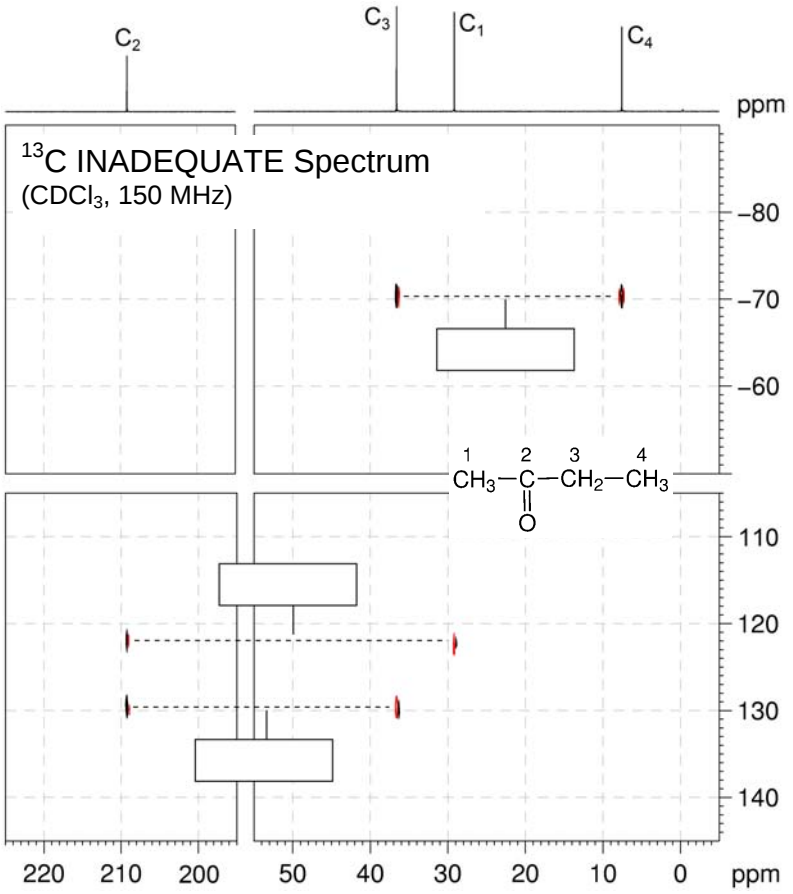
$^{13}C\{^{1}H\}$ NMR Spectrum
($CDCl_3$, 100 MHz)




H1
H3
H4
ppm
1H–1H COSY Spectrum
(CDCl3, 400 MHz)
H4
H1
H3
1.0
1.5
2.0
2.5
3.0
3.0
2.5
2.0
1.5
1.0
ppm


H1
H3
H4
ppm
1H–13C me-HSQC Spectrum
(CDCl3, 400 MHz)
C4
C1
C3
5
10
15
20
25
30
35
40
45
1 2 3 4
CH3—C—CH2—CH3
O
3.0
2.5
2.0
1.5
1.0
ppm


H1
H3
H4
ppm
1H–13C HMBC Spectrum
(CDCl3, 400 MHz)
C4
C1
C3
C2
0
10
20
30
40
50
200
210
220
3.0
2.5
2.0
1.5
1.0
ppm


C2
C3
C1
C4
ppm
13C INADEQUATE Spectrum
(CDCl3, 150 MHz)
–80
–70
–60
1 2 3 4
CH3—C—CH2—CH3
O
110
120
130
140
220
210
200
50
40
30
20
10
0
ppm