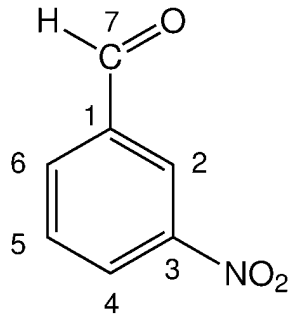
Problem 12

The ^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of 3-nitrobenzaldehyde ($C_7H_5NO_3$) recorded in $CDCl_3$ solution at 298 K and 500 MHz are given below.

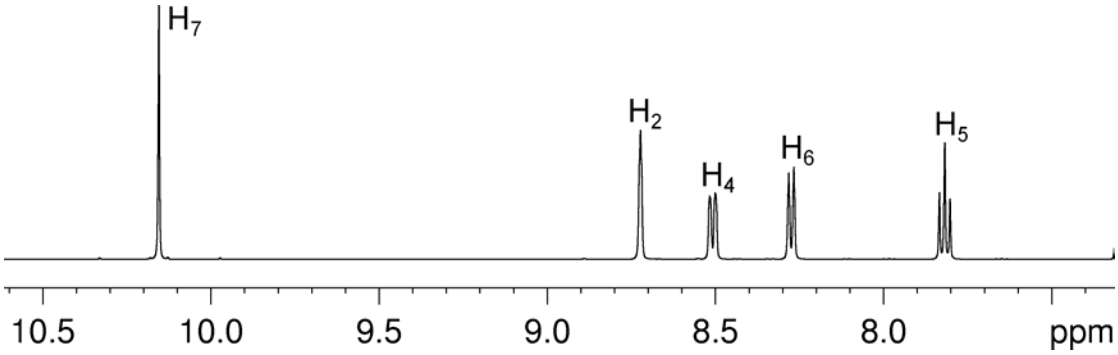
The ^{1}H NMR spectrum has signals at δ 7.82 (H_5), 8.28 (H_6), 8.51 (H_4), 8.73 (H_2) and 10.15 (H_7) ppm.

The $^{13}C\{^{1}H\}$ NMR spectrum has signals at δ 124.4 (C_2), 128.6 (C_4), 130.5 (C_5), 134.8 (C_6), 137.5 (C_1), 148.8 (C_3) and 189.9 (C_7) ppm.

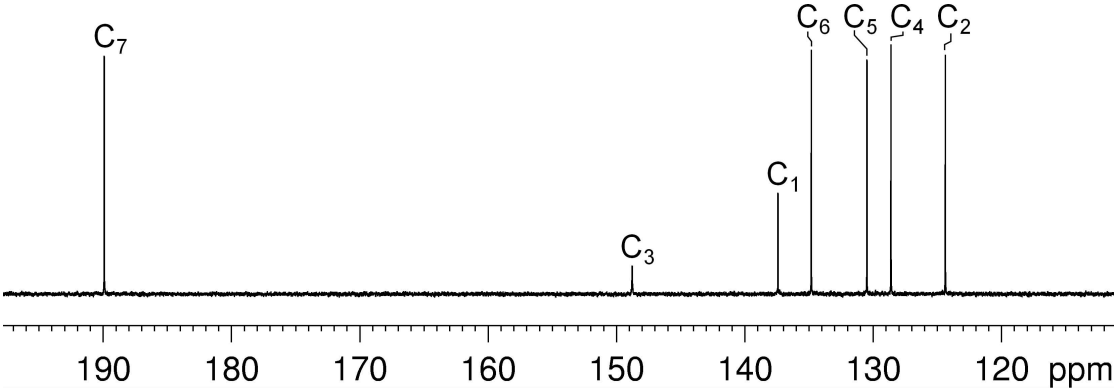
Also given on the following pages are the ^{1}H–^{1}H COSY, ^{1}H–^{13}C me-HSQC, ^{1}H–^{13}C HMBC, ^{1}H–^{1}H NOESY and INADEQUATE spectra. For each 2D spectrum, indicate which correlation gives rise to each cross-peak by placing an appropriate label in the box provided.

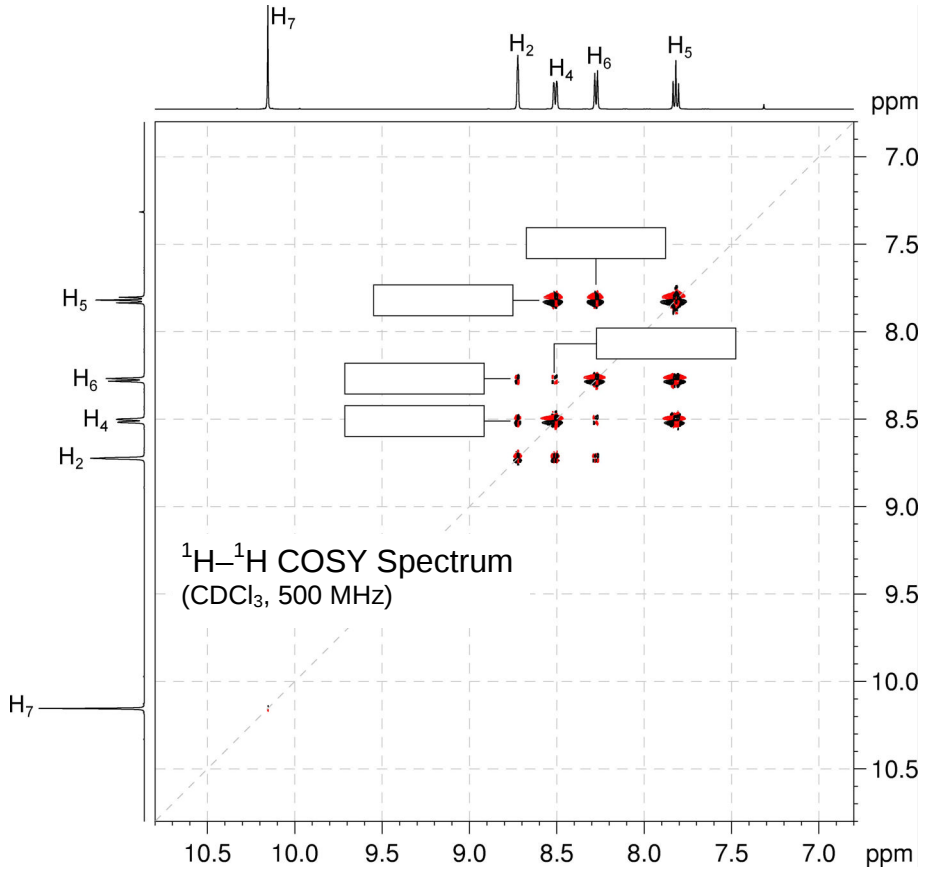


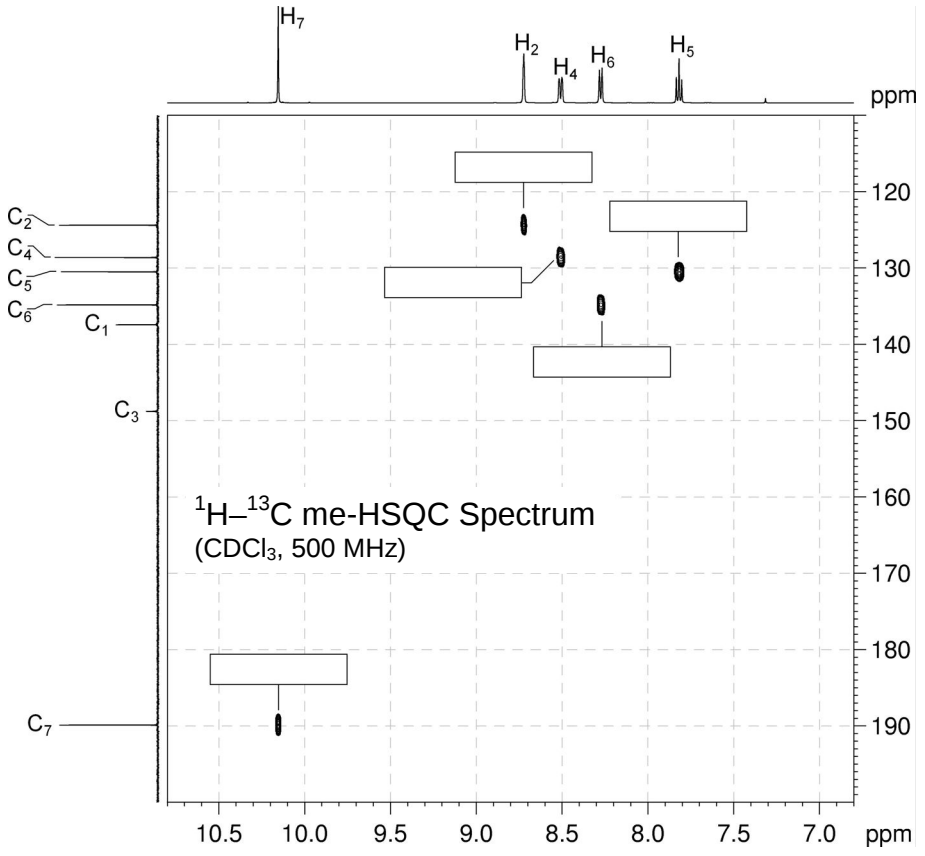
^{1}H NMR Spectrum
($CDCl_3$, 500 MHz)

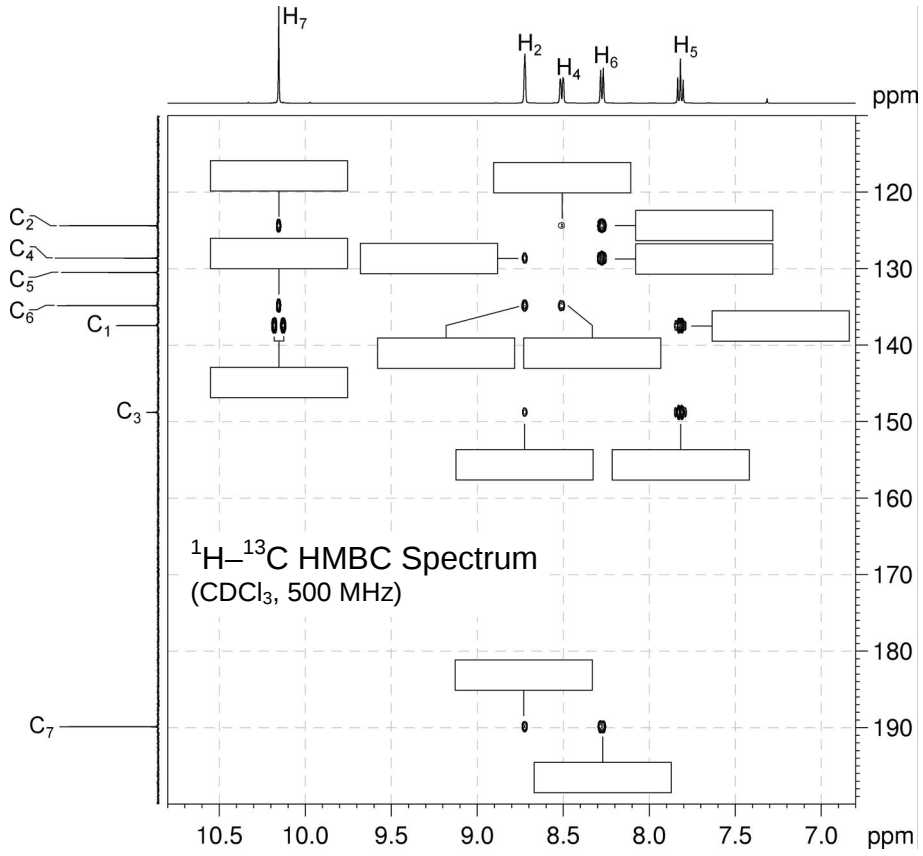


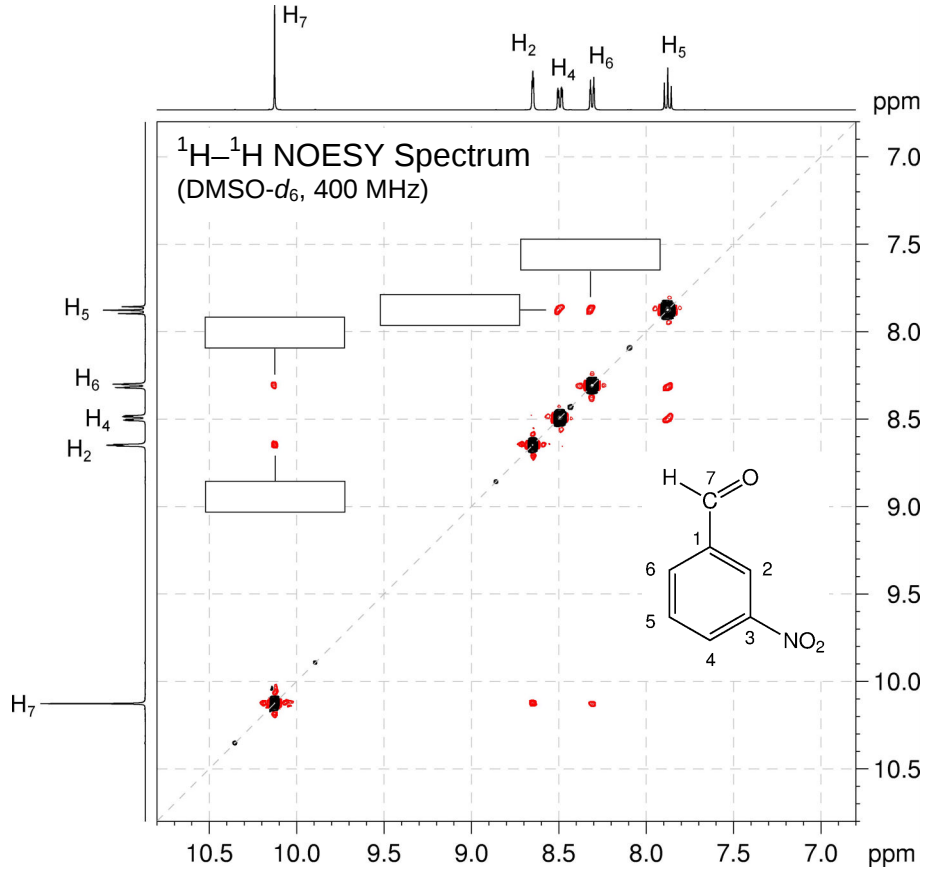
$^{13}C\{^{1}H\}$ NMR Spectrum
($CDCl_3$, 125 MHz)

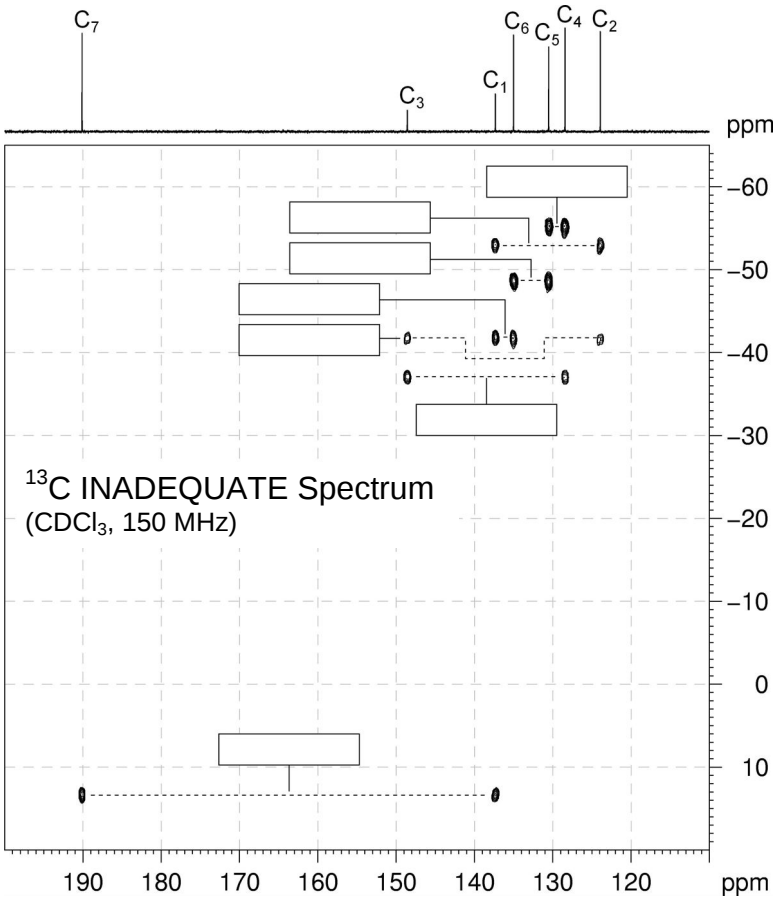


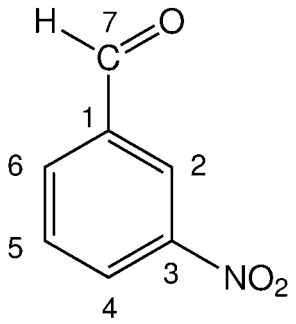

H7
H2
H4
H6
H5
ppm
7.0
7.5
8.0
8.5
9.0
9.5
10.0
10.5
H5
H6
H4
H2
H7
1H–1H COSY Spectrum
(CDCl3, 500 MHz)
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
ppm


H7
H2
H4
H6
H5
ppm
120
130
140
150
160
170
180
190
C2
C4
C5
C6
C1
C3
C7
1H–13C me-HSQC Spectrum
(CDCl3, 500 MHz)
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
ppm


H7
H2
H4
H6
H5
ppm
C2
C4
C5
C6
C1
C3
C7
120
130
140
150
160
170
180
190
1H–13C HMBC Spectrum
(CDCl3, 500 MHz)
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
ppm


H7
H2
H4
H6
H5
ppm
1H–1H NOESY Spectrum
(DMSO-d6, 400 MHz)
H5
H6
H4
H2
H7
7.0
7.5
8.0
8.5
9.0
9.5
10.0
10.5
H
7
O
C
1
2
3
4
5
6
NO2
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
ppm


C7
C3
C1
C6
C5
C4
C2
ppm
–60
–50
–40
–30
–20
–10
0
10
190
180
170
160
150
140
130
120
ppm
13C INADEQUATE Spectrum
(CDCl3, 150 MHz)


H
7
O
C
1
6
2
5
3
NO2
4