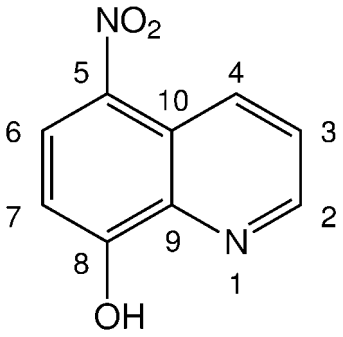
Problem 14

The ^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of 8-hydroxy-5-nitroquinoline ($C_9H_6N_2O_3$) recorded in DMSO-d_6 solution at 298 K and 400 MHz are given below.

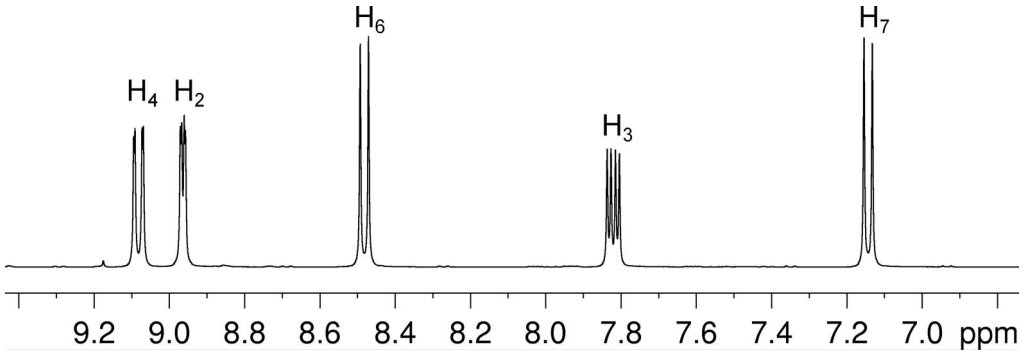
The ^{1}H NMR spectrum has signals at δ 7.14 (H_7), 7.82 (H_3), 8.48 (H_6), 8.97 (H_2) and 9.08 (H_4) ppm. The hydroxyl proton is not shown.

The $^{13}C\{^{1}H\}$ NMR spectrum has signals at δ 110.0 (C_7), 122.5 (C_{10}), 125.2 (C_3), 129.1 (C_6), 132.4 (C_4), 135.0 (C_5), 137.2 (C_9), 149.1 (C_2) and 160.7 (C_8) ppm.

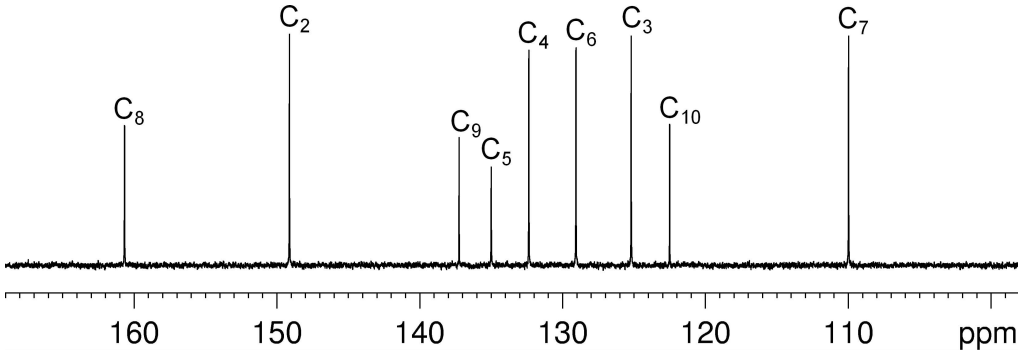
Also given on the following pages are the ^{1}H–^{1}H COSY, ^{1}H–^{13}C me-HSQC, ^{1}H–^{13}C HMBC and INADEQUATE spectra. For each 2D spectrum, indicate which correlation gives rise to each cross-peak by placing an appropriate label in the box provided.

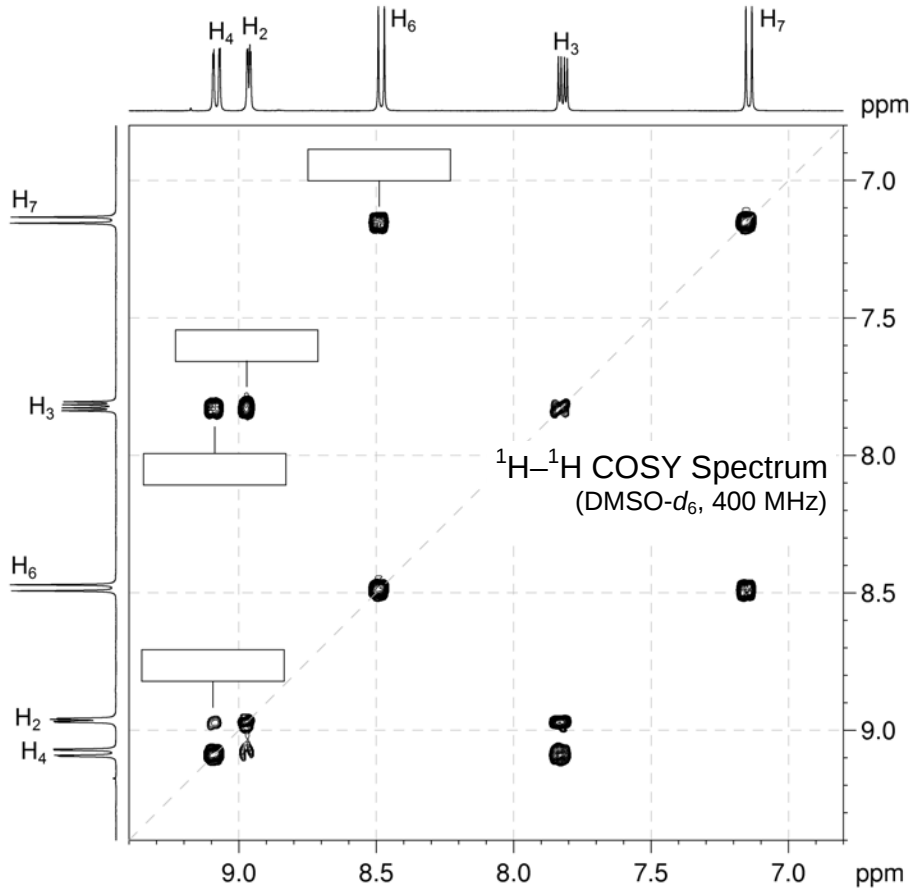


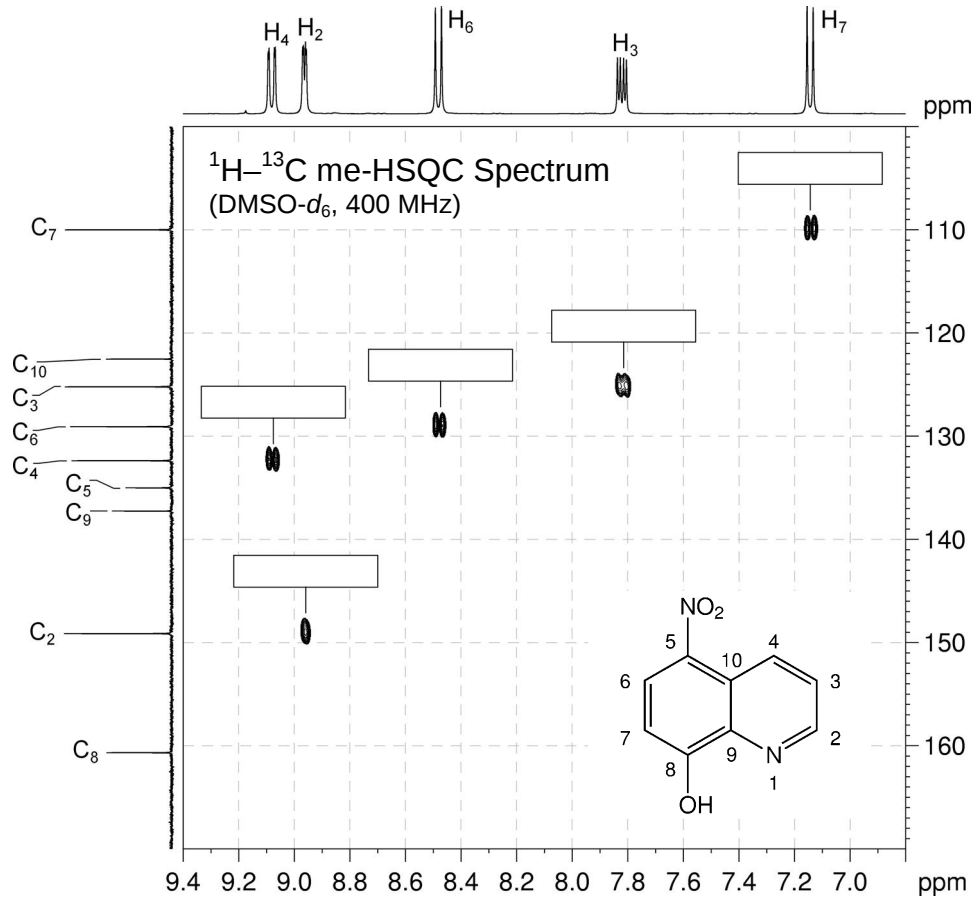
^{1}H NMR Spectrum
(DMSO-d_6, 400 MHz)

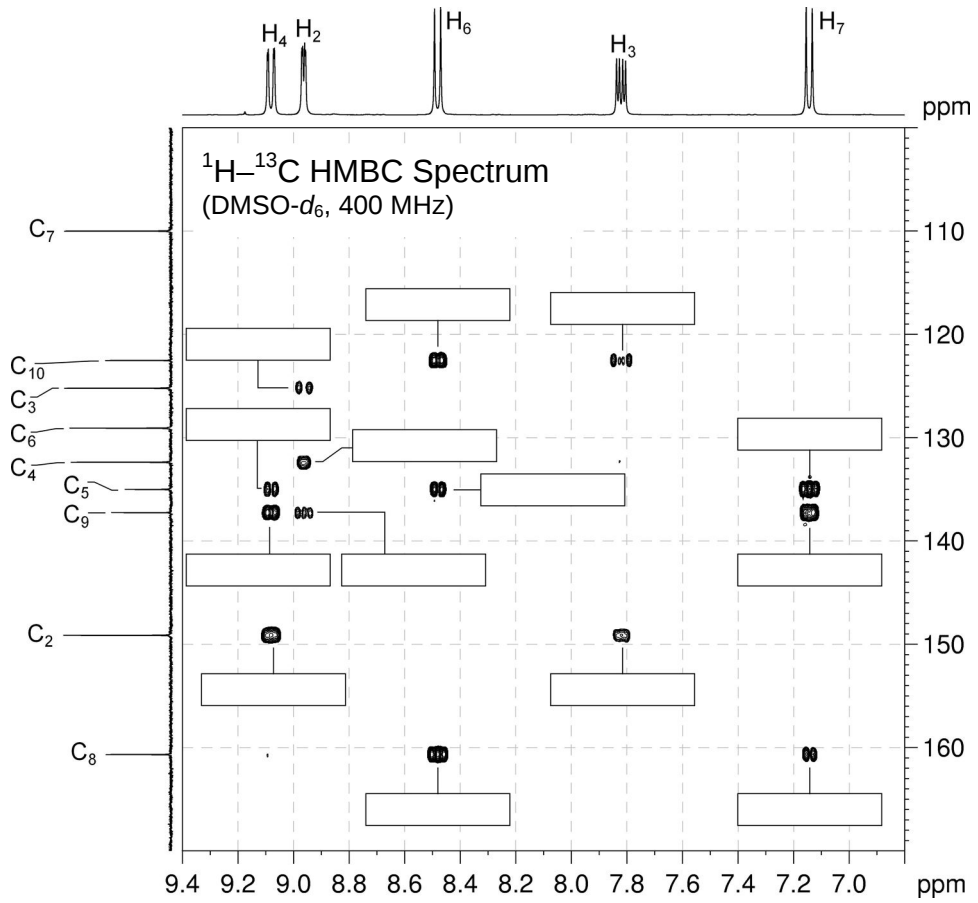


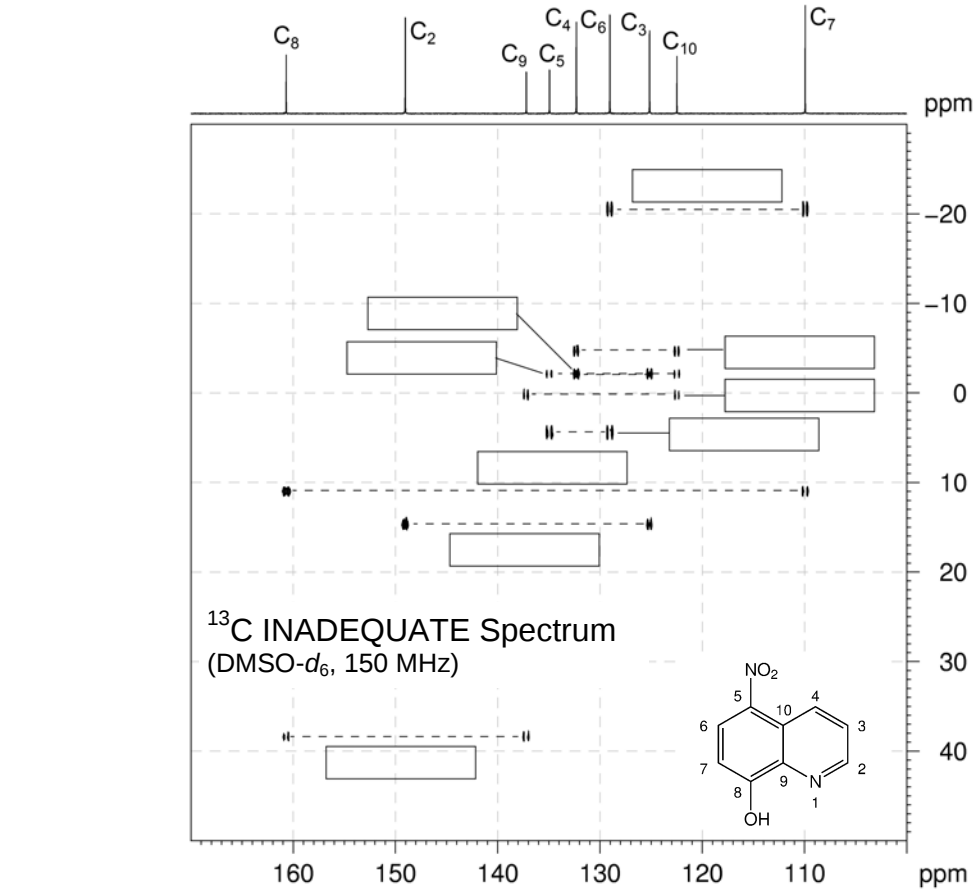
$^{13}C\{^{1}H\}$ NMR Spectrum
(DMSO-d_6, 100 MHz)




H4 H2
H6
H3
H7
ppm
H7
H3
H6
H2
H4
7.0
7.5
8.0
8.5
9.0
9.0
8.5
8.0
7.5
7.0
ppm
1H–1H COSY Spectrum
(DMSO-d6, 400 MHz)


H4 H2
H6
H3
H7
ppm
1H–13C me-HSQC Spectrum
(DMSO-d6, 400 MHz)
C7
C10
C3
C6
C4
C5
C9
C2
C8
110
120
130
140
150
160
9.4 9.2 9.0 8.8 8.6 8.4 8.2 8.0 7.8 7.6 7.4 7.2 7.0
ppm
NO2
OH
N


H4 H2
H6
H3
H7
ppm
1H–13C HMBC Spectrum
(DMSO-d6, 400 MHz)
C7
C10
C3
C6
C4
C5
C9
C2
C8
110
120
130
140
150
160
9.4 9.2 9.0 8.8 8.6 8.4 8.2 8.0 7.8 7.6 7.4 7.2 7.0
ppm


C8
C2
C9 C5
C4 C6 C3
C10
C7
ppm
–20
–10
0
10
20
30
40
13C INADEQUATE Spectrum
(DMSO-d6, 150 MHz)
NO2
OH
N
160 150 140 130 120 110
ppm