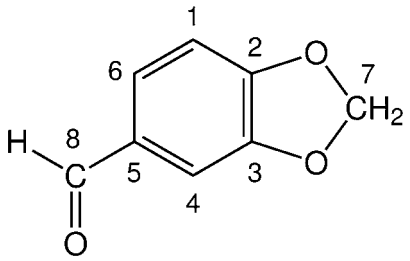
Problem 29

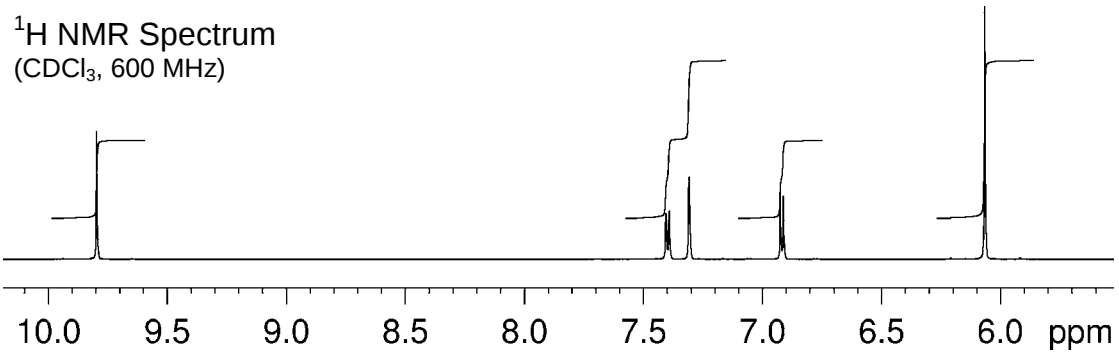
The ^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of piperonal ($C_8H_6O_3$) recorded in $CDCl_3$ solution at 298 K and 600 MHz are given below.

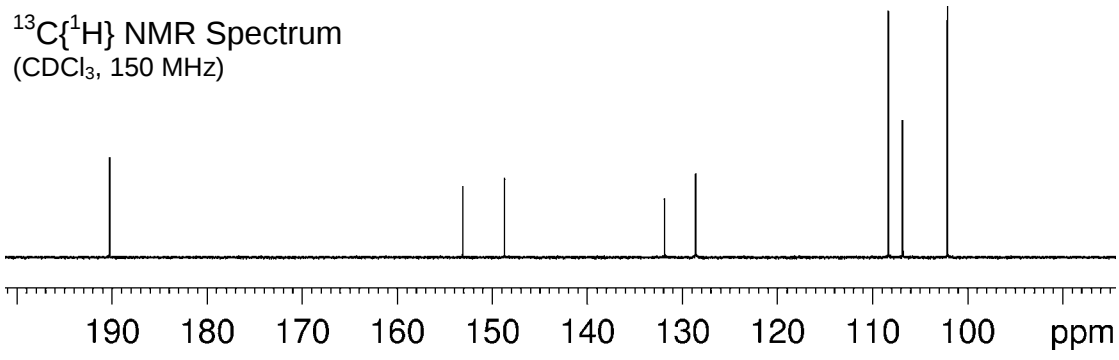
The ^{1}H NMR spectrum has signals at δ 6.07 (s, 2H, H_7), 6.92 (d, $^{3}J_{HH}$ = 7.9 Hz, 1H, H_1), 7.31 (d, $^{4}J_{HH}$ = 1.5 Hz, 1H, H_4), 7.40 (dd, $^{3}J_{HH}$ = 7.9 Hz, $^{4}J_{HH}$ = 1.5 Hz, 1H, H_6) and 9.80 (s, 1H, H_8) ppm.

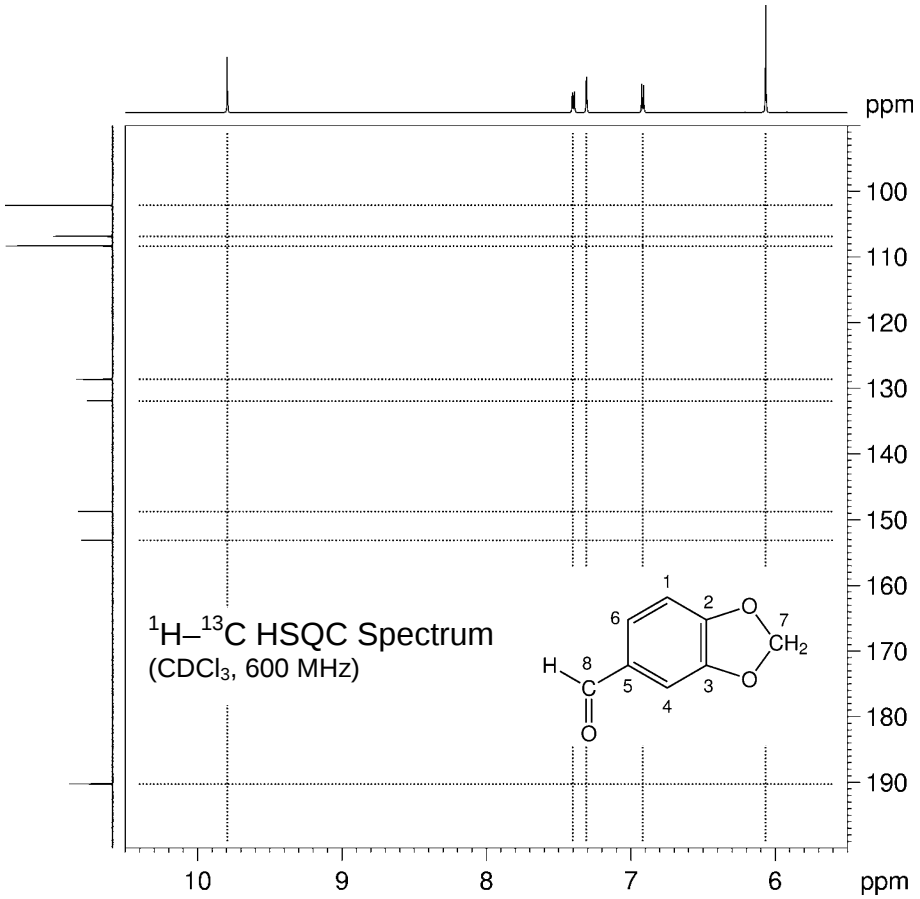
The $^{13}C\{^{1}H\}$ NMR spectrum has signals at δ 102.1 (C_7), 106.9 (C_4), 108.3 (C_1), 128.6 (C_6), 131.9 (C_5), 148.7 (C_3), 153.1 (C_2) and 190.2 (C_8) ppm.

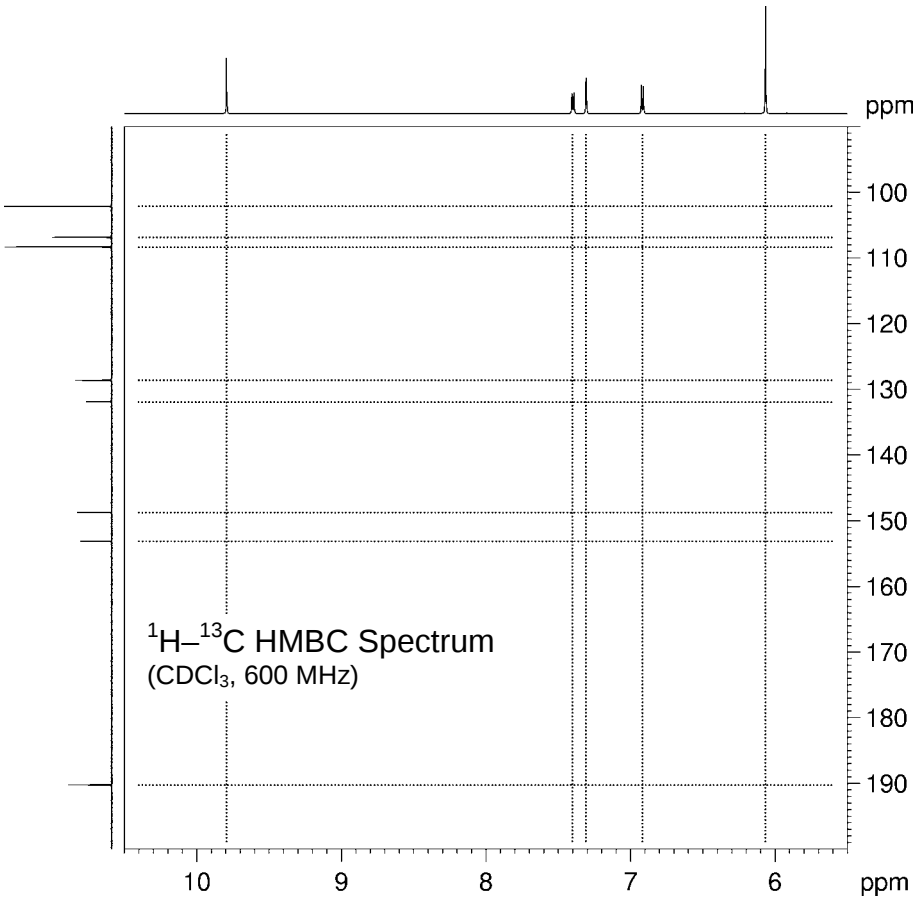
Use this information to produce schematic diagrams of the HSQC and HMBC spectra, showing where all of the cross-peaks and diagonal peaks would be.








ppm
100
110
120
130
140
150
160
170
180
190
10
9
8
7
6
ppm
$^{1}H–^{13}C$ HSQC Spectrum
($CDCl_3$, 600 MHz)
1
2
O
7
CH_2
O
3
4
5
6
H
8
C
O


ppm
100
110
120
130
140
150
160
170
180
190
10
9
8
7
6
ppm
$^{1}H–^{13}C$ HMBC Spectrum
($CDCl_3$, 600 MHz)