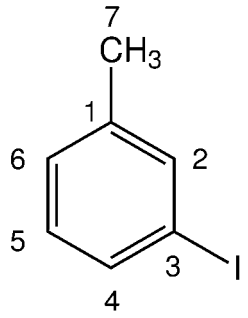
Problem 13

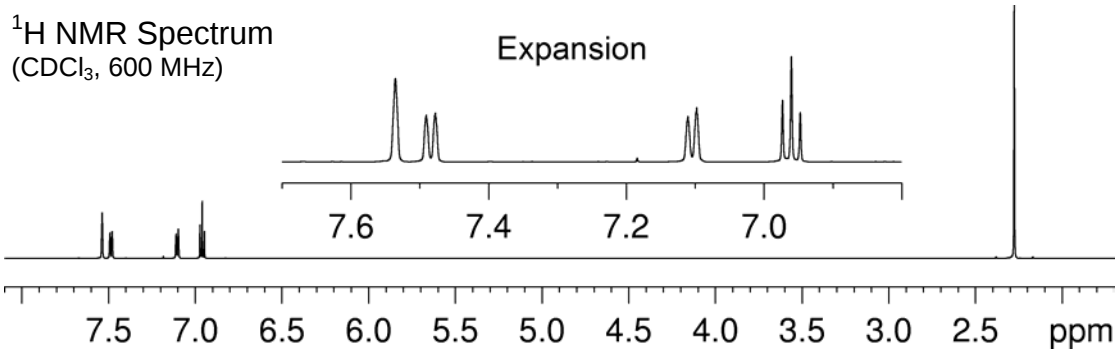
The ^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of 3-iodotoluene (C_7H_6I) recorded in $CDCl_3$ solution at 298 K and 600 MHz are given below.

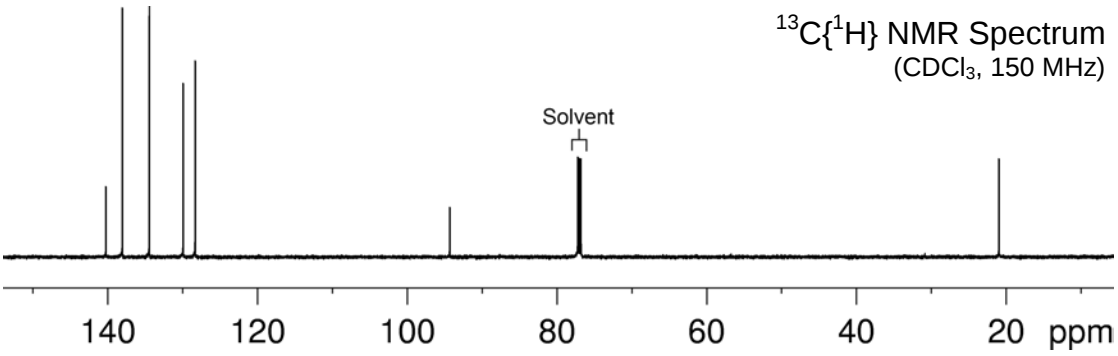
The ^{1}H NMR spectrum has signals at δ 2.28 (H_7), 6.96 (H_5), 7.11 (H_6), 7.48 (H_4) and 7.53 (H_2) ppm.

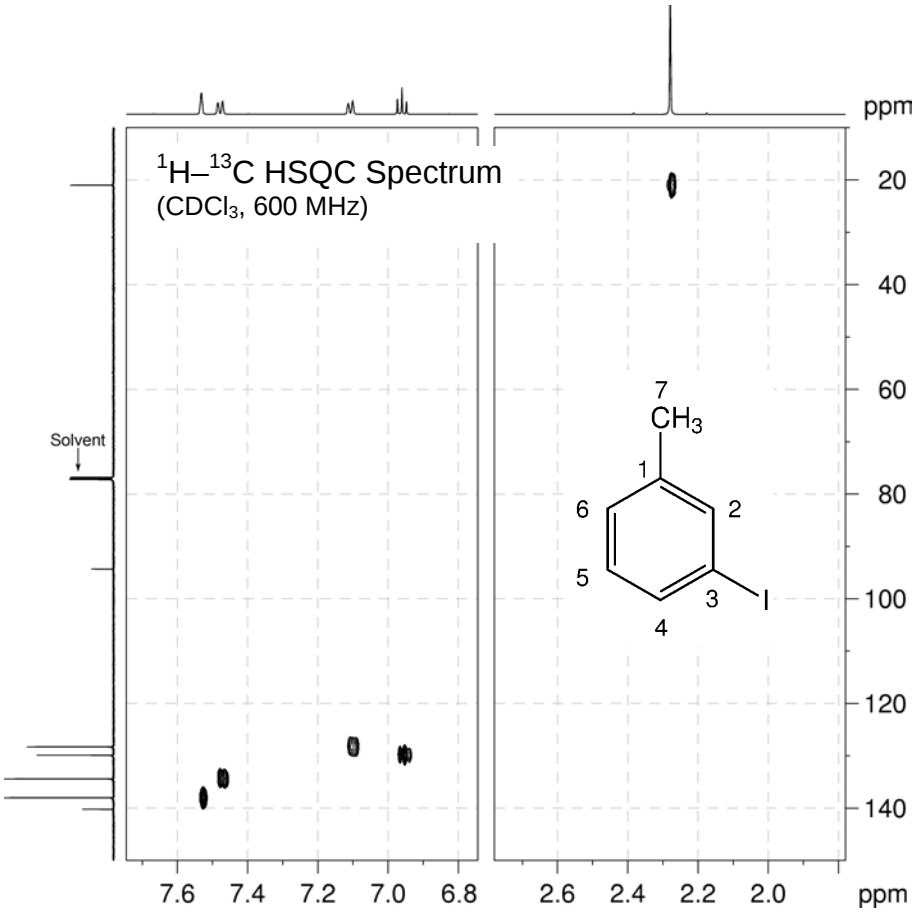
The $^{13}C\{^{1}H\}$ NMR spectrum has signals at δ 21.0, 94.3, 128.3, 129.9, 134.4, 138.0 and 140.2 ppm.

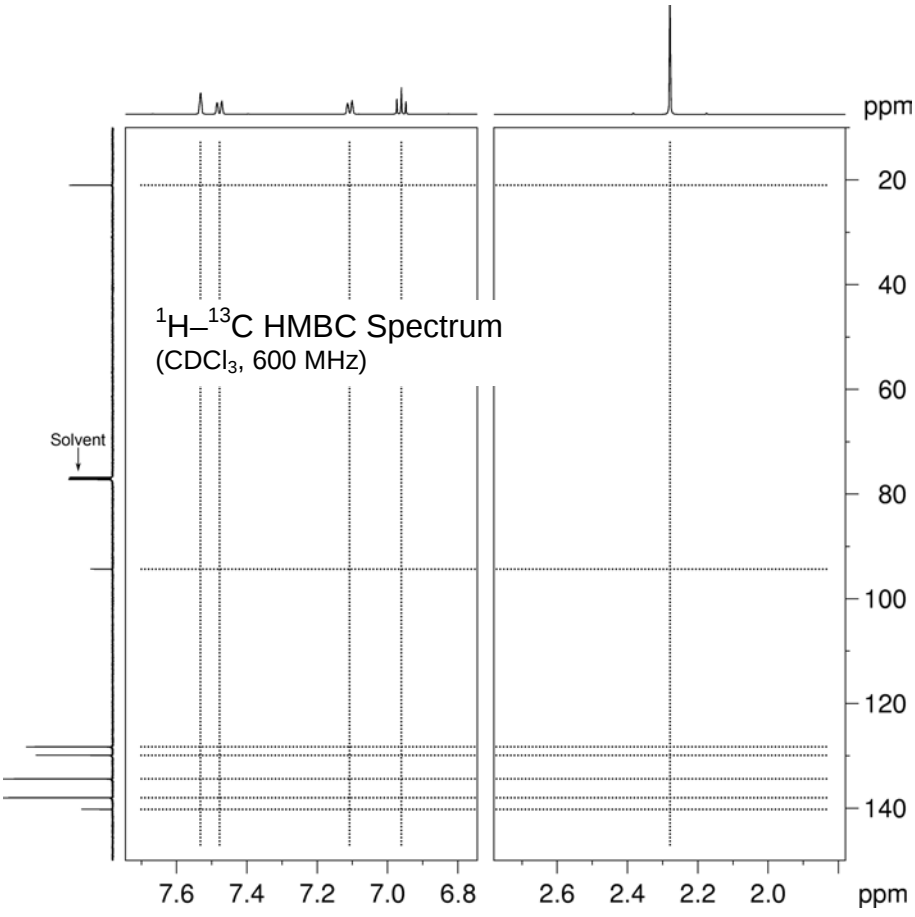
Use the me-HSQC spectrum to assign the protonated carbon signals, and then use this information to produce a schematic HMBC spectrum, showing where all of the cross-peaks would be.








^{1}H–^{13}C HSQC Spectrum
(CDCl$_3$, 600 MHz)
Solvent
7
CH$_3$
1
2
3
I
4
5
6
ppm
20
40
60
80
100
120
140
7.6
7.4
7.2
7.0
6.8
2.6
2.4
2.2
2.0
ppm


^{1}H–^{13}C HMBC Spectrum
(CDCl$_3$, 600 MHz)
Solvent
ppm
20
40
60
80
100
120
140
7.6
7.4
7.2
7.0
6.8
2.6
2.4
2.2
2.0
ppm