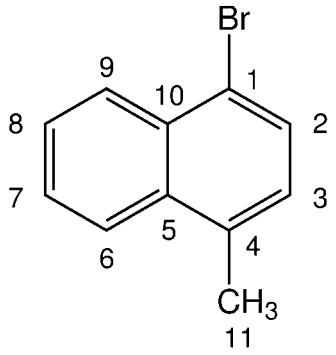
Problem 52

The ^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of 1-bromo-4-methylnaphthalene ($C_{11}H_9Br$) recorded in $CDCl_3$ solution at 298 K and 500 MHz are given below.

The ^{1}H NMR spectrum has signals at δ 2.58, 7.08, 7.50, 7.54, 7.61, 7.91 and 8.23 ppm.

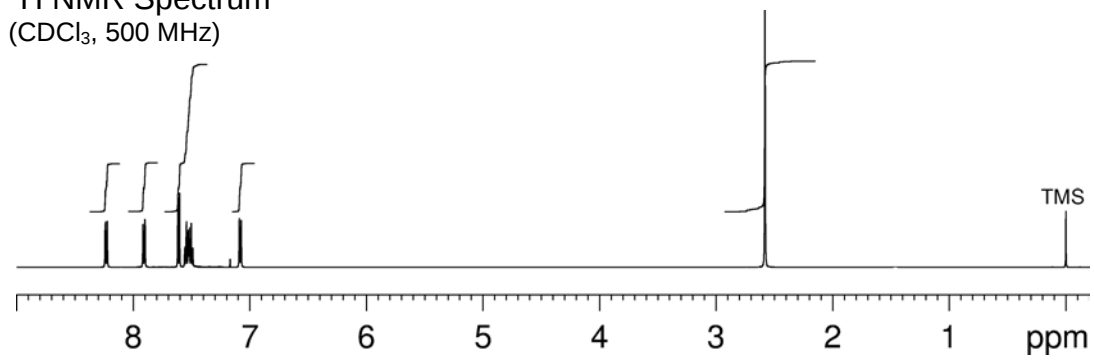
The $^{13}C\{^{1}H\}$ NMR spectrum has signals at δ 19.2, 120.6, 124.5, 126.4, 126.85, 126.91, 127.6, 129.4, 131.7, 133.7 and 134.3 ppm.

The 2D ^{1}H–^{1}H COSY, multiplicity-edited ^{1}H–^{13}C HSQC and ^{1}H–^{13}C HMBC spectra are given on the following pages. Use these spectra to assign the ^{1}H and $^{13}C\{^{1}H\}$ resonances for this compound.

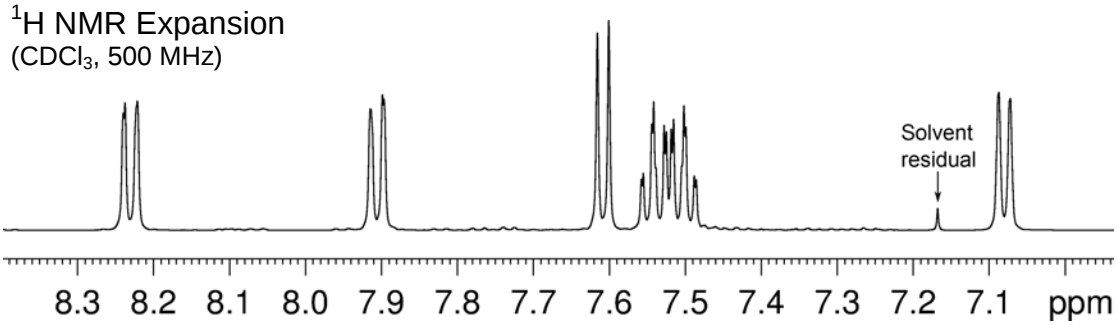


Proton	Chemical Shift (ppm)	Carbon	Chemical Shift (ppm)
		C_1	
H_2		C_2	
H_3		C_3	
		C_4	
		C_5	
H_6		C_6	
H_7		C_7	
H_8		C_8	
H_9		C_9	
		C_{10}	
H_{11}		C_{11}	

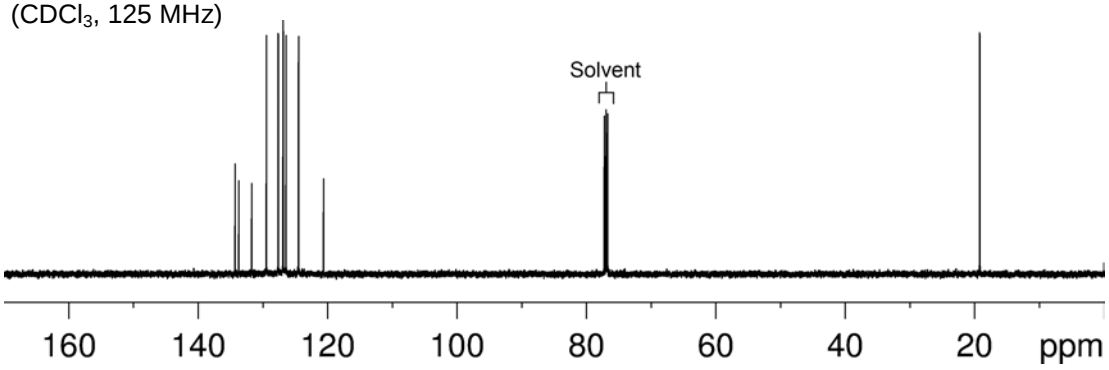
^{1}H NMR Spectrum
($CDCl_3$, 500 MHz)



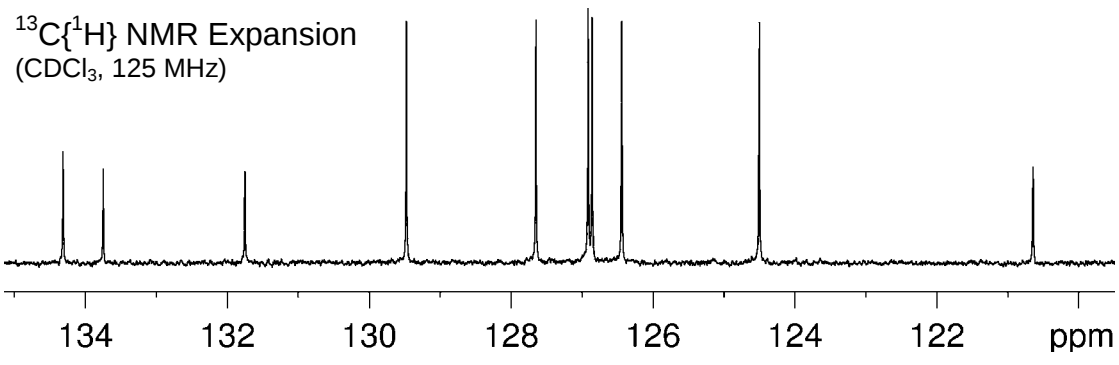
^{1}H NMR Expansion
($CDCl_3$, 500 MHz)

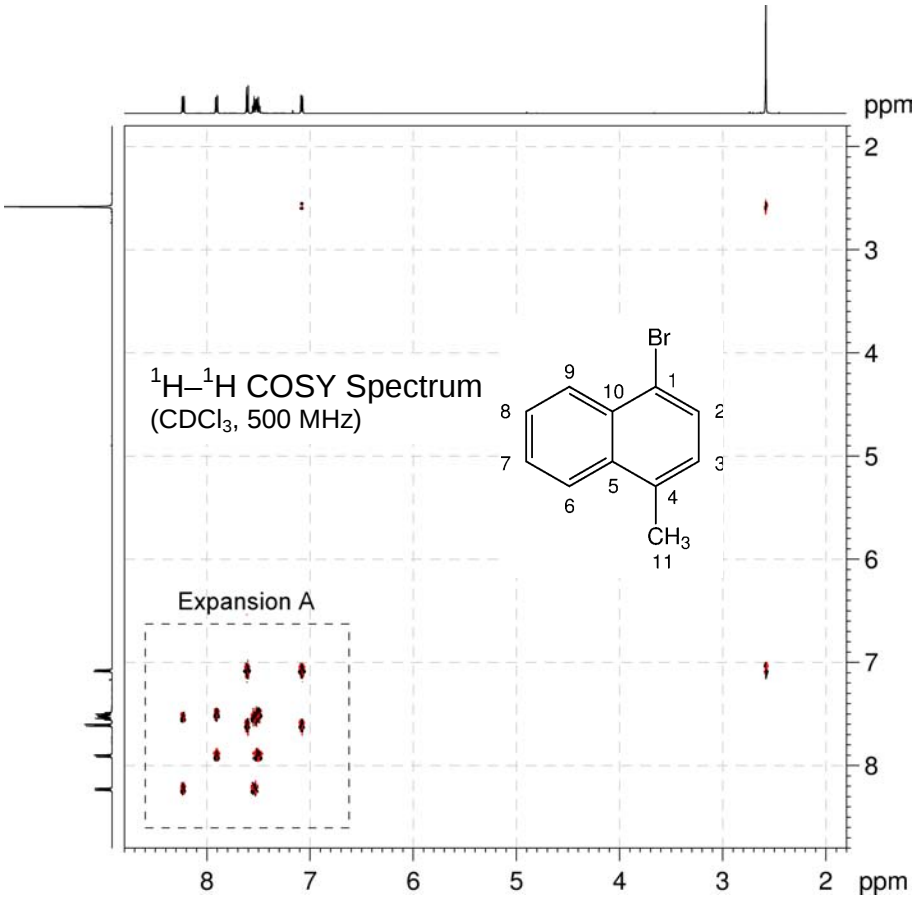


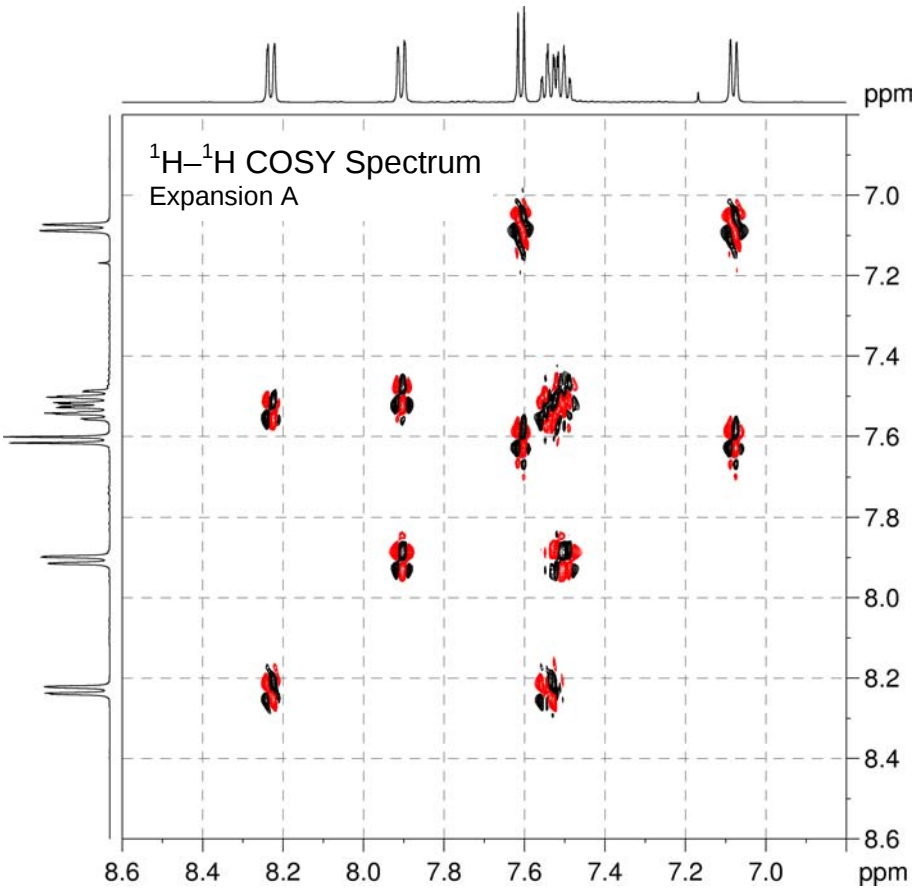
^{13}C{^{1}H} NMR Spectrum
($CDCl_3$, 125 MHz)

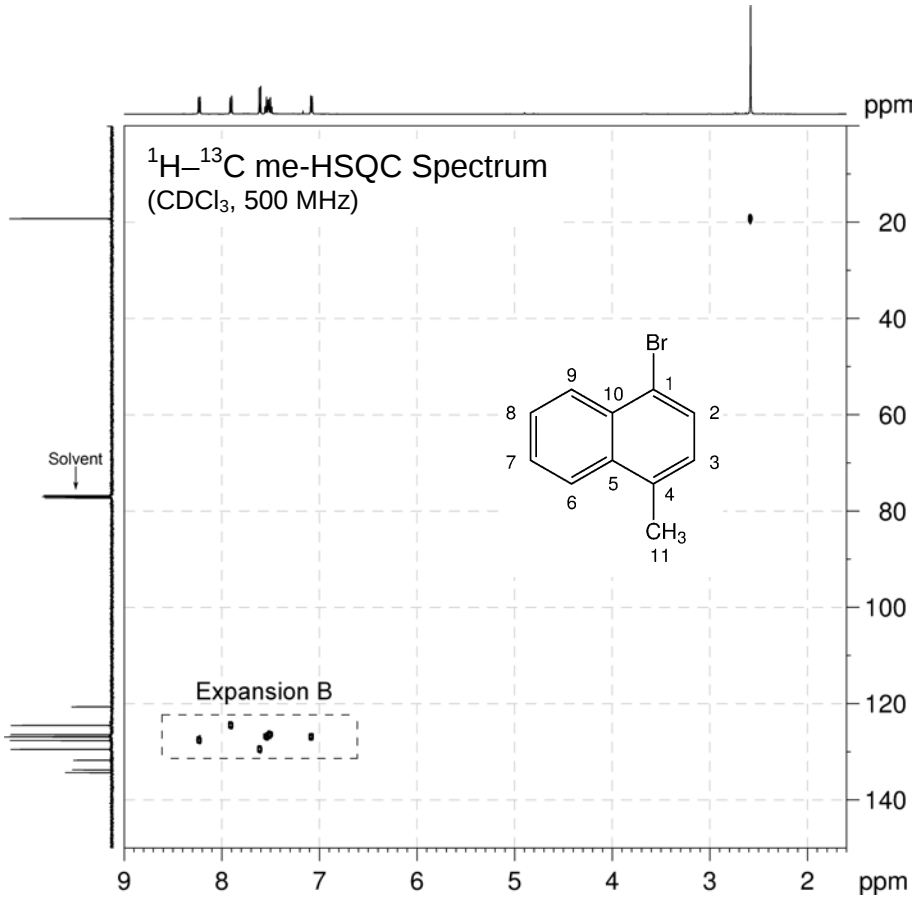


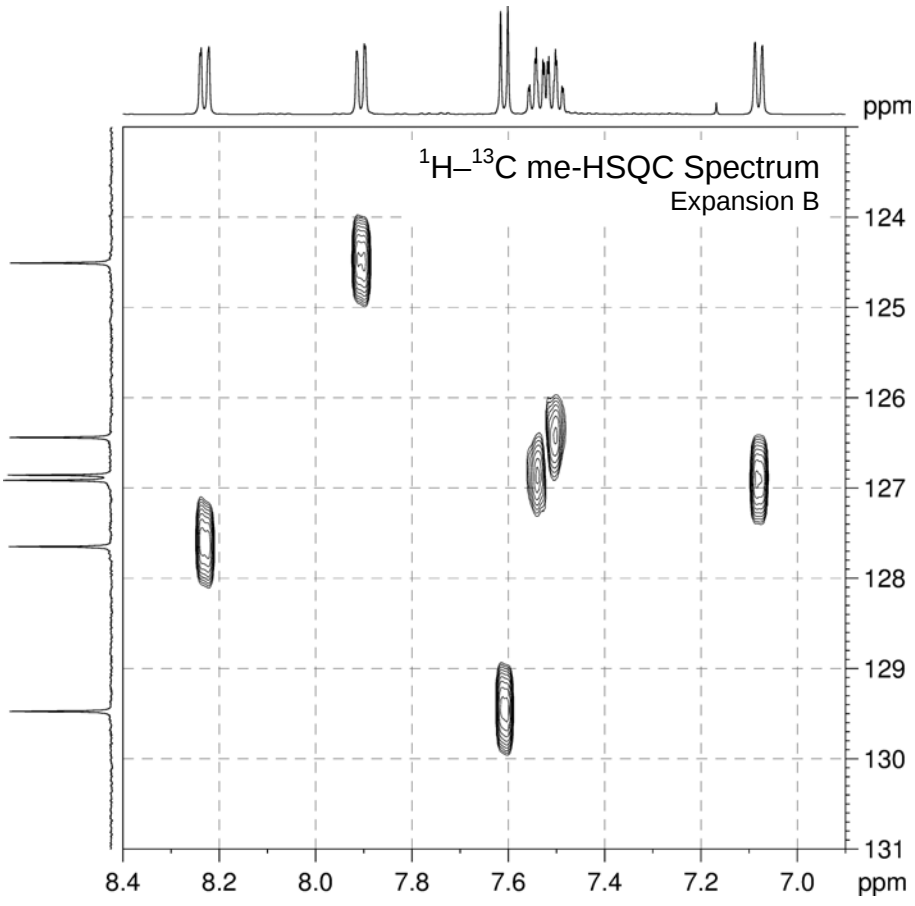
^{13}C{^{1}H} NMR Expansion
($CDCl_3$, 125 MHz)

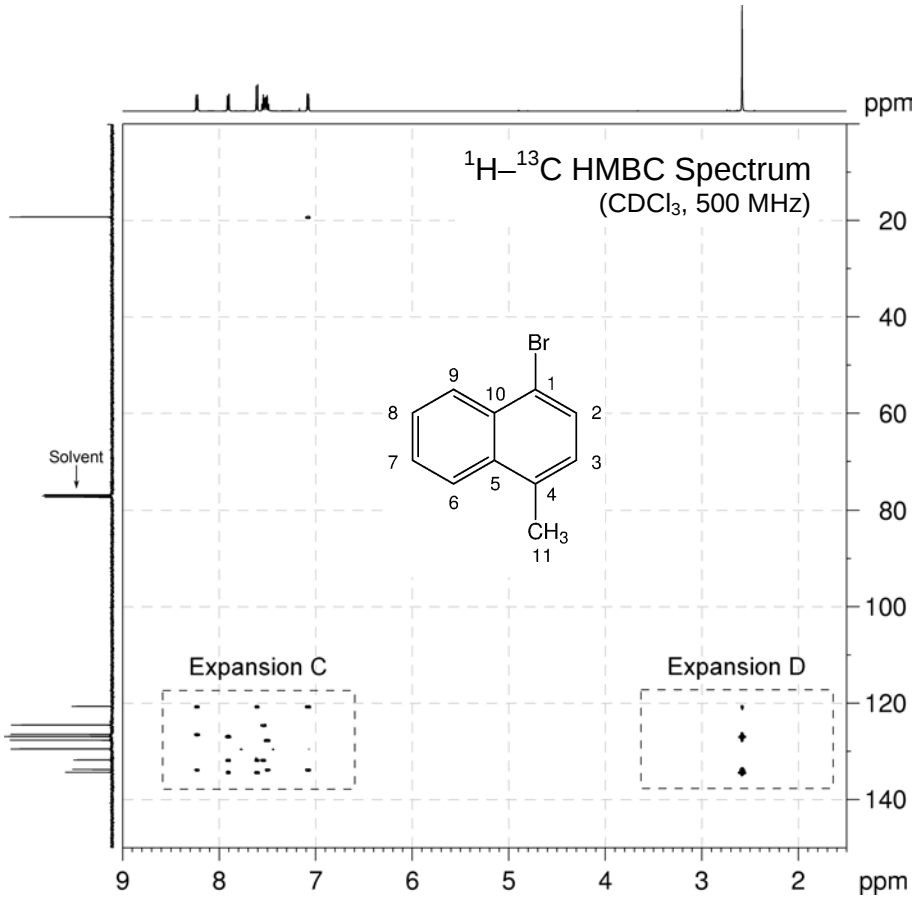


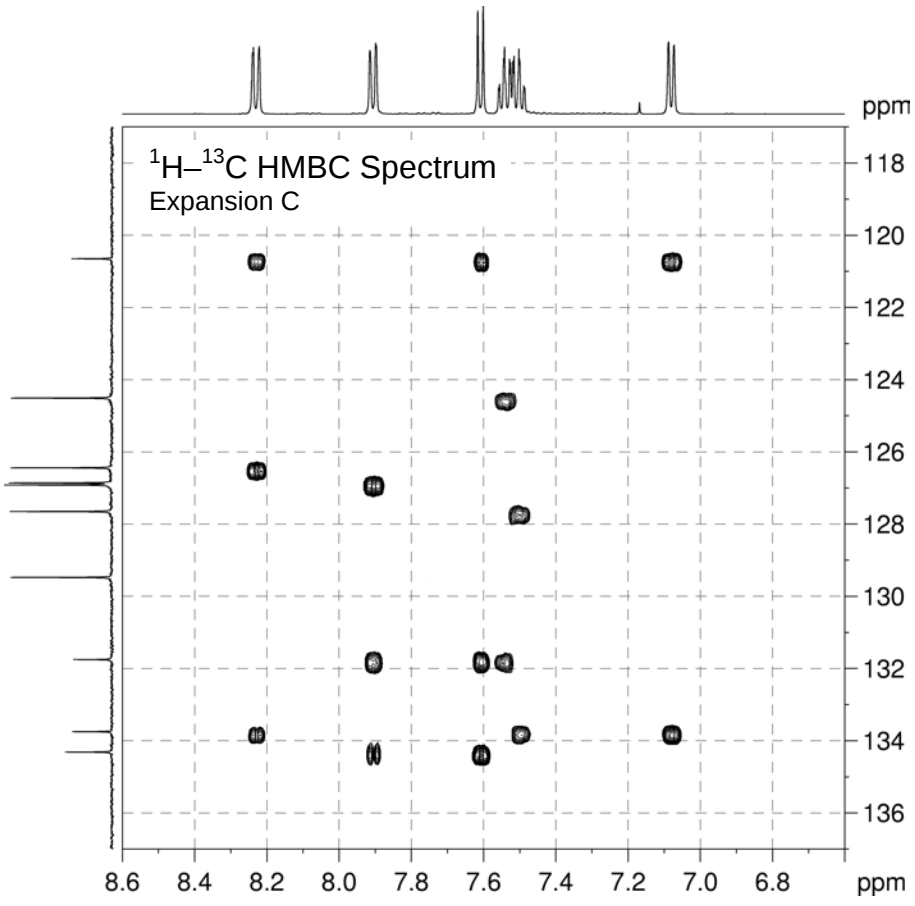

^{1}H–^{1}H COSY Spectrum
(CDCl$_3$, 500 MHz)
Br
CH$_3$
Expansion A
ppm

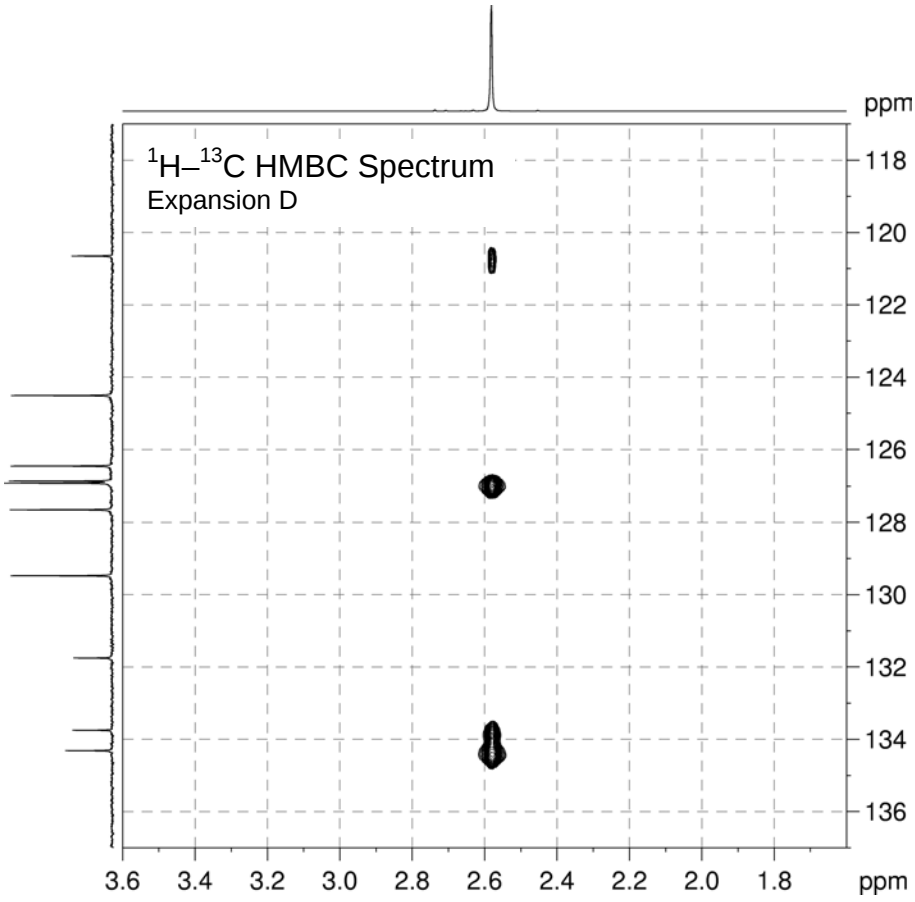

^{1}H–^{1}H COSY Spectrum
Expansion A
ppm

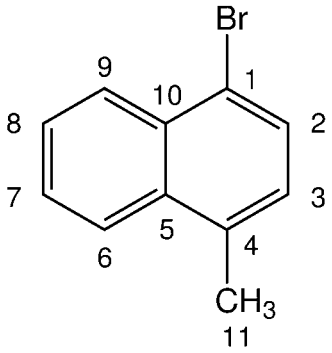

^{1}H–^{13}C me-HSQC Spectrum
(CDCl$_3$, 500 MHz)
Solvent
Expansion B
Br
CH$_3$
ppm
20
40
60
80
100
120
140
9
8
7
6
5
4
3
2
ppm


^{1}H–^{13}C me-HSQC Spectrum
Expansion B
ppm
124
125
126
127
128
129
130
131
8.4
8.2
8.0
7.8
7.6
7.4
7.2
7.0
ppm


^{1}H–^{13}C HMBC Spectrum
(CDCl$_3$, 500 MHz)
Br
CH$_3$
Solvent
Expansion C
Expansion D
ppm


^{1}H–^{13}C HMBC Spectrum
Expansion C
ppm


^{1}H–^{13}C HMBC Spectrum
Expansion D
ppm
118
120
122
124
126
128
130
132
134
136
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
ppm


Br
1
2
3
4
5
6
7
8
9
10
CH3
11