6 Problems

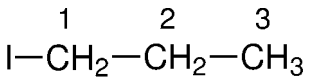
Problem 1

The ^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of 1-iodopropane (C_3H_7I) recorded in $CDCl_3$ solution at 298 K and 400 MHz are given below.

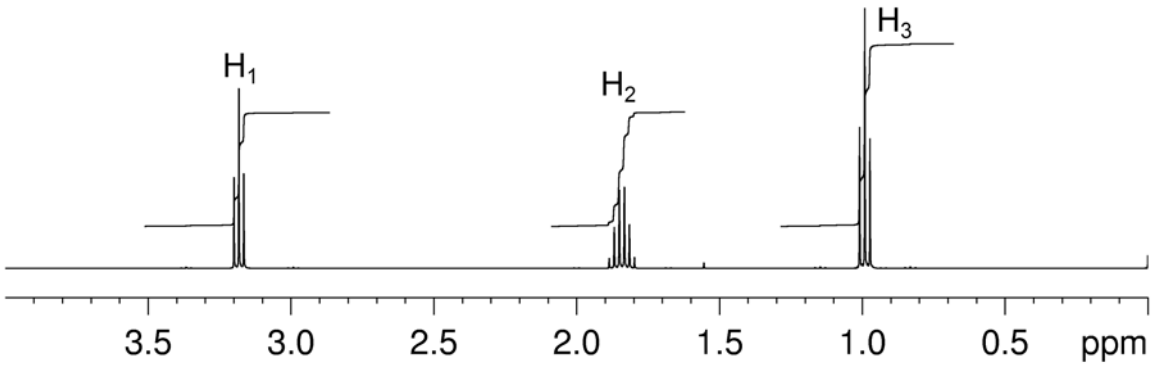
The ^{1}H NMR spectrum has signals at δ 0.99 (H_3), 1.84 (H_2) and 3.18 (H_1) ppm.

The $^{13}C\{^{1}H\}$ NMR spectrum has signals at δ 9.6 (C_1), 15.3 (C_3) and 26.9 (C_2) ppm.

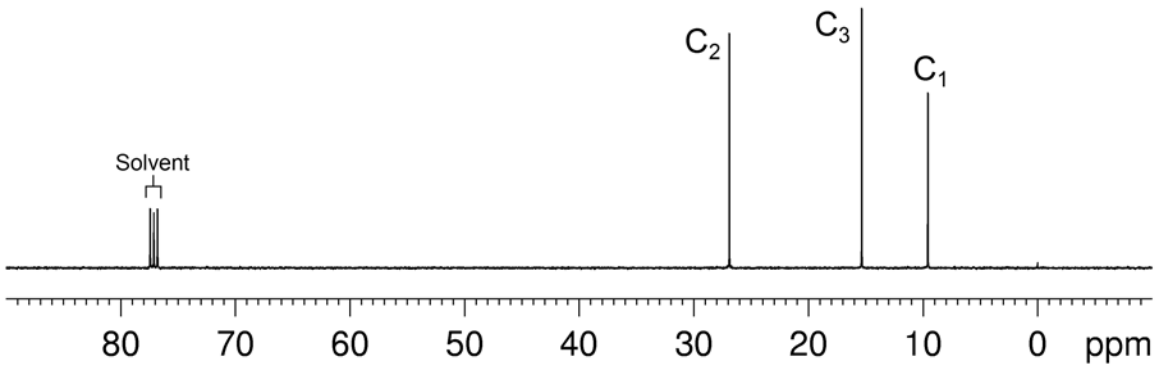
Also given on the following pages are the ^{1}H–^{1}H COSY, ^{1}H–^{13}C me-HSQC, ^{1}H–^{13}C HMBC and INADEQUATE spectra. For each 2D spectrum, indicate which correlation gives rise to each cross-peak by placing an appropriate label in the box provided (*e.g.* $H_1 \rightarrow H_2$, $H_1 \rightarrow C_1$).

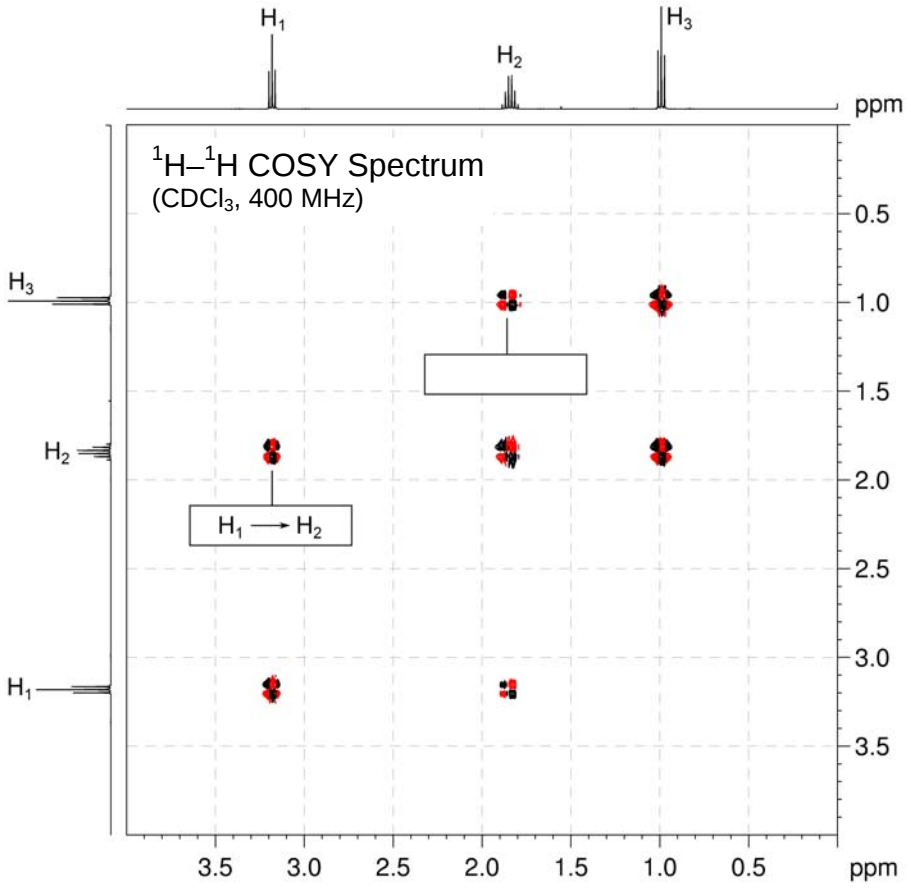


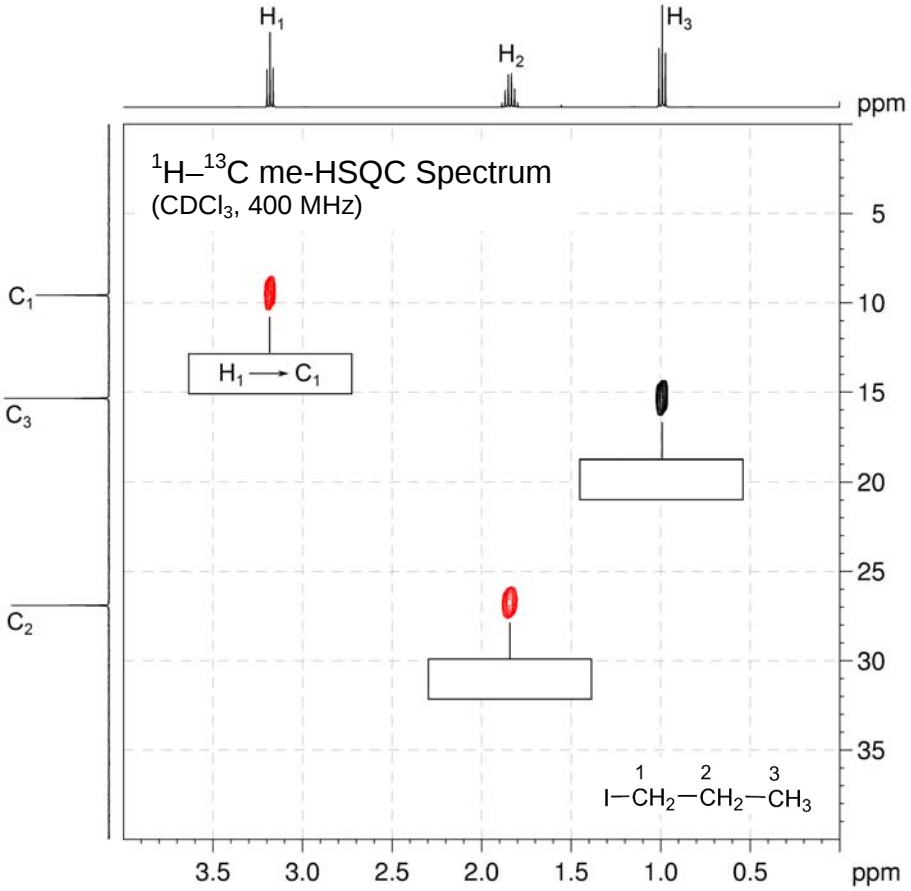
^{1}H NMR Spectrum
($CDCl_3$, 400 MHz)

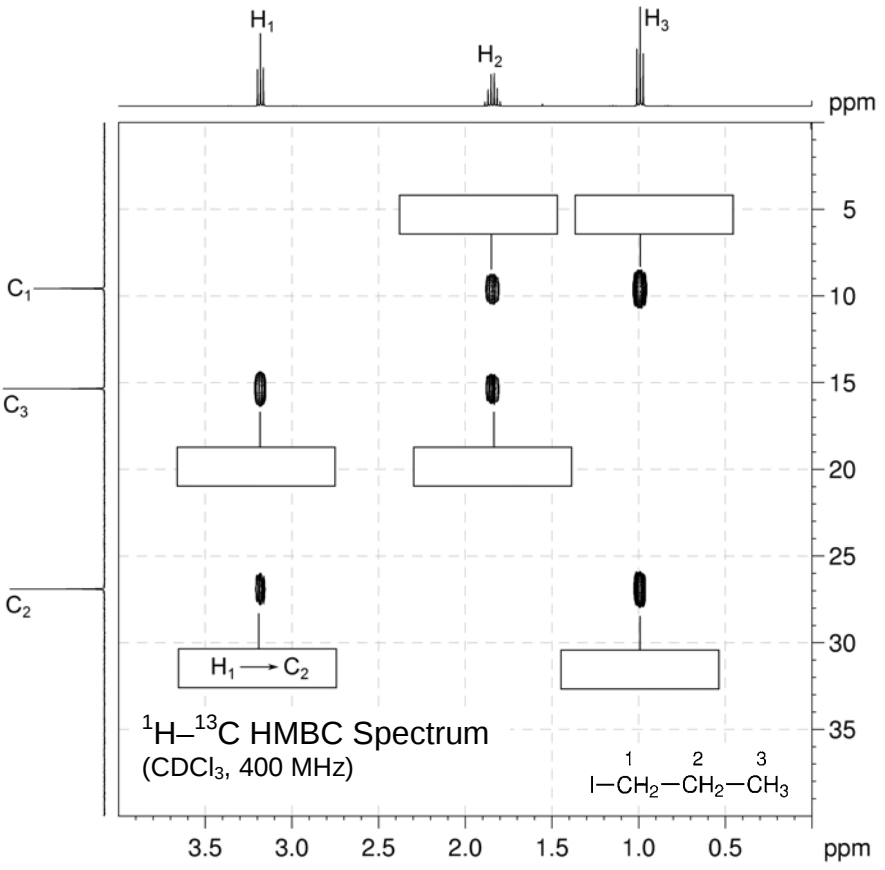


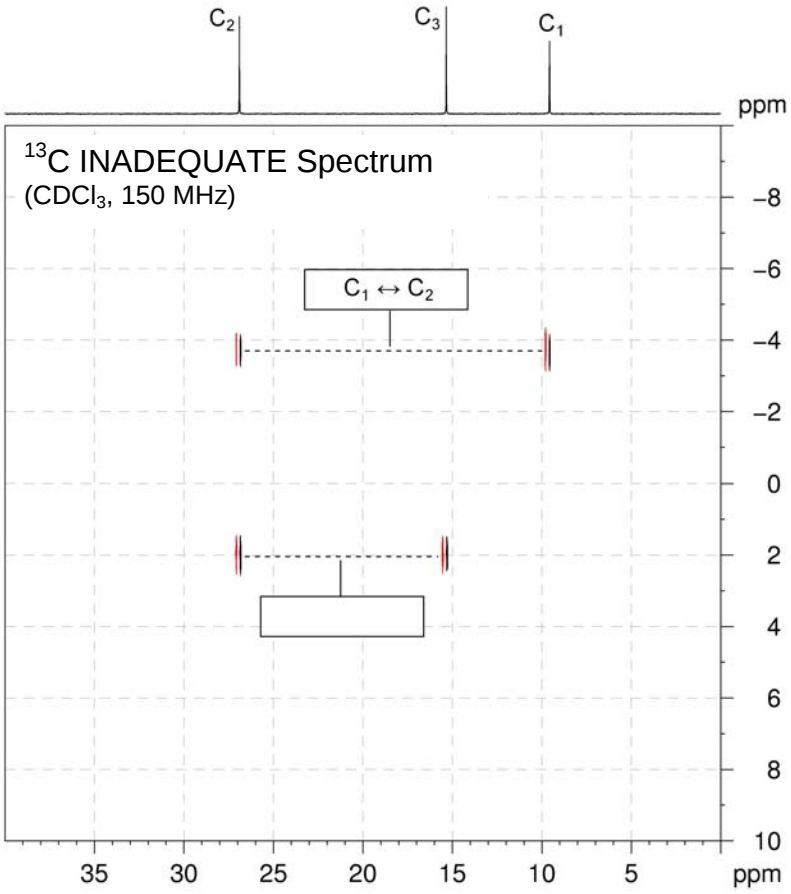
$^{13}C\{^{1}H\}$ NMR Spectrum
($CDCl_3$, 100 MHz)




H1
H2
H3
ppm
1H–1H COSY Spectrum
(CDCl3, 400 MHz)
H3
H2
H1
H1 → H2
0.5
1.0
1.5
2.0
2.5
3.0
3.5
3.5 3.0 2.5 2.0 1.5 1.0 0.5
ppm


H1
H2
H3
ppm
1H–13C me-HSQC Spectrum
(CDCl3, 400 MHz)
C1
C3
C2
H1 → C1
5
10
15
20
25
30
35
1 2 3
I—CH2—CH2—CH3
3.5 3.0 2.5 2.0 1.5 1.0 0.5
ppm


H1
H2
H3
ppm
C1
C3
C2
5
10
15
20
25
30
35
H1 → C2
1H–13C HMBC Spectrum
(CDCl3, 400 MHz)
1 2 3
I—CH2—CH2—CH3
3.5 3.0 2.5 2.0 1.5 1.0 0.5
ppm


C2
C3
C1
ppm
13C INADEQUATE Spectrum
(CDCl3, 150 MHz)
C1 ↔ C2
–8
–6
–4
–2
0
2
4
6
8
10
35 30 25 20 15 10 5
ppm