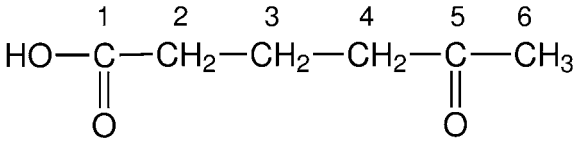
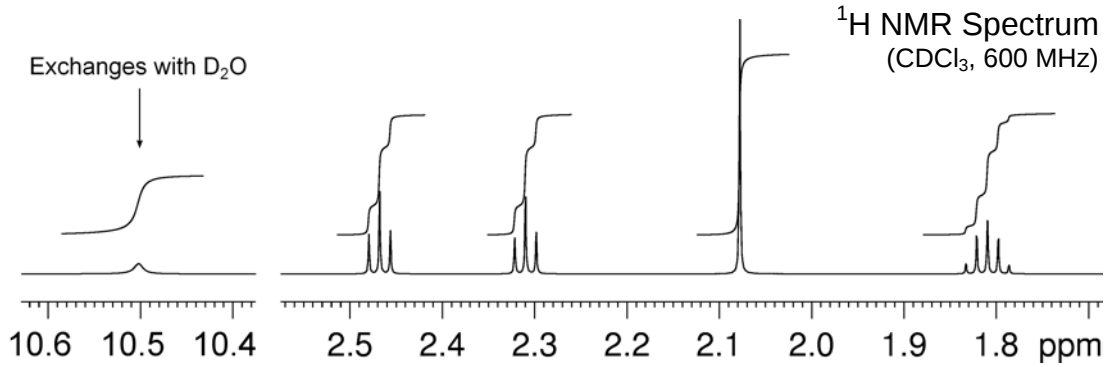
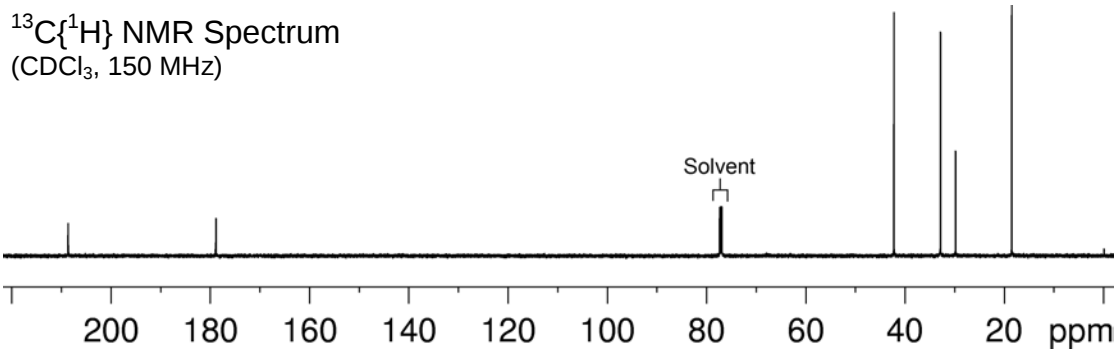
# Problem 6

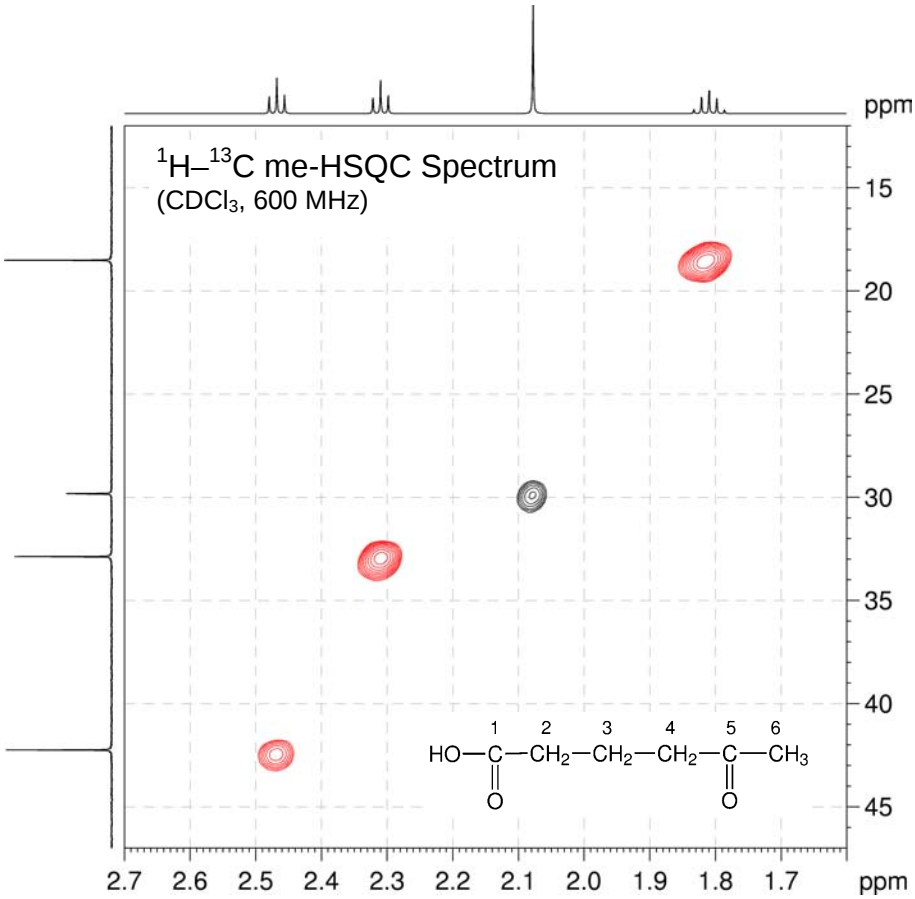
The $^{1}H$ and $^{13}C\{^{1}H\}$ NMR spectra of 4-acetylbutyric acid ($C_6H_{10}O_3$) recorded in $CDCl_3$ solution at 298 K and 600 MHz are given below. The $^{1}H$ NMR spectrum has signals at $\delta$ 1.81, 2.08, 2.31, 2.47 and 10.5 ppm. The $^{13}C\{^{1}H\}$ NMR spectrum has signals at $\delta$ 18.5, 29.8, 32.9, 42.2, 178.8 and 208.6 ppm. The $^{1}H$–$^{13}C$ me-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.

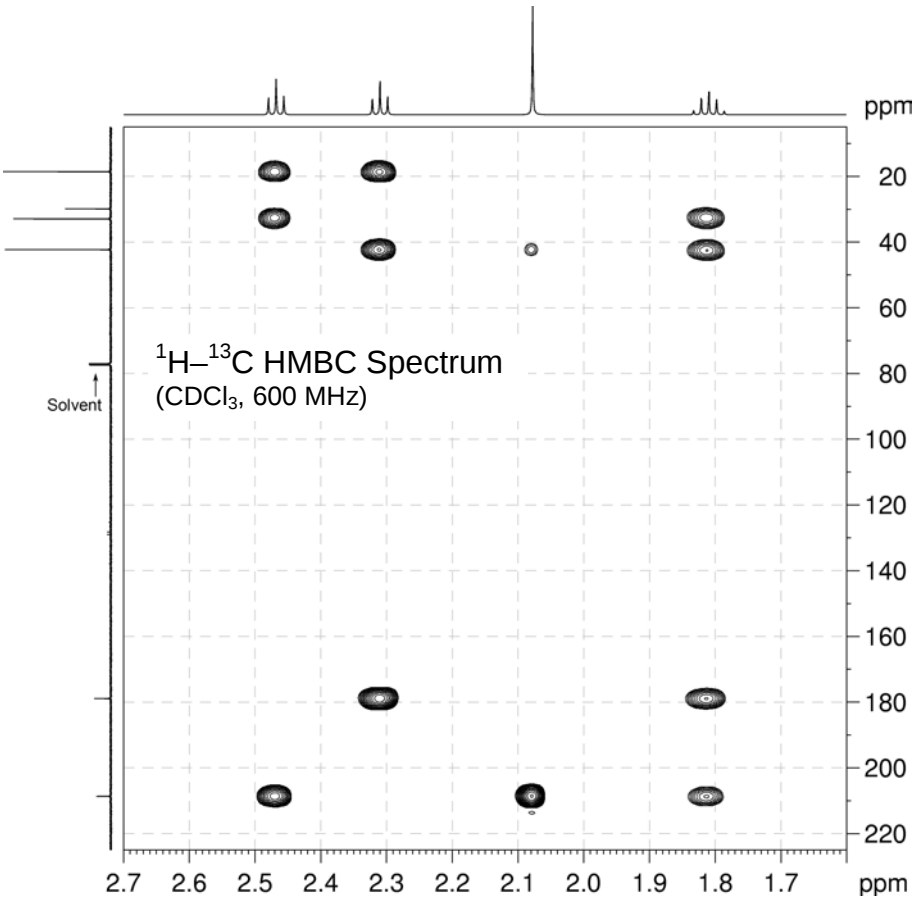



| Proton | Chemical Shift (ppm) | Carbon | Chemical Shift (ppm) |
|---|---|---|---|
| | | $C_1$ | |
| $H_2$ | | $C_2$ | |
| $H_3$ | | $C_3$ | |
| $H_4$ | | $C_4$ | |
| | | $C_5$ | |
| $H_6$ | | $C_6$ | |
| OH | | | |


$^{1}H$–$^{13}C$ me-HSQC Spectrum
($CDCl_3$, 600 MHz)
ppm
15
20
25
30
35
40
45
2.7 2.6 2.5 2.4 2.3 2.2 2.1 2.0 1.9 1.8 1.7
ppm
HO—C—CH2—CH2—CH2—C—CH3
1 2 3 4 5 6
O
O


$^{1}H$–$^{13}C$ HMBC Spectrum
($CDCl_3$, 600 MHz)
Solvent
ppm
20
40
60
80
100
120
140
160
180
200
220
2.7 2.6 2.5 2.4 2.3 2.2 2.1 2.0 1.9 1.8 1.7
ppm