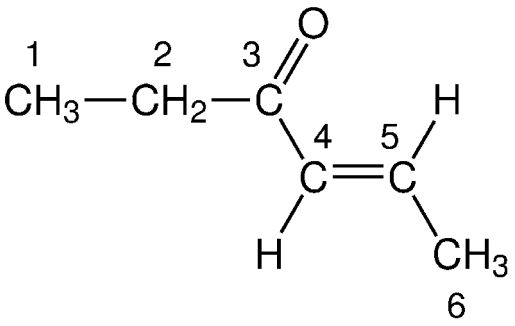
Problem 10

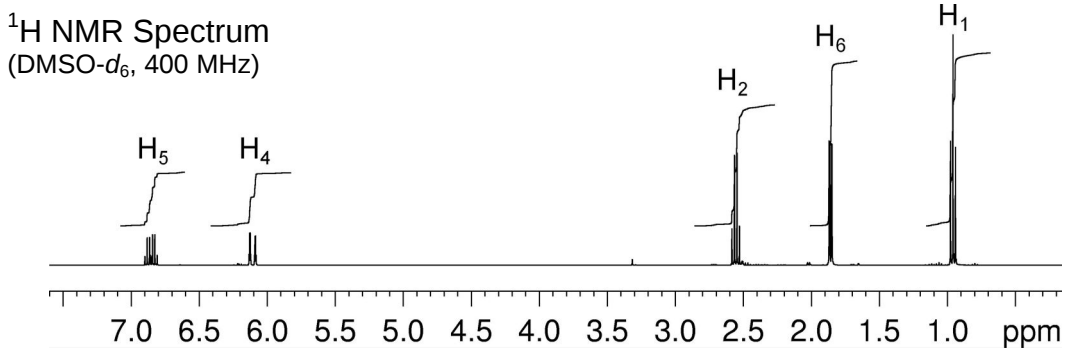
The ^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of *trans*-4-hexen-3-one ($C_6H_{10}O$) recorded in DMSO-d_6 solution at 298 K and 400 MHz are given below.

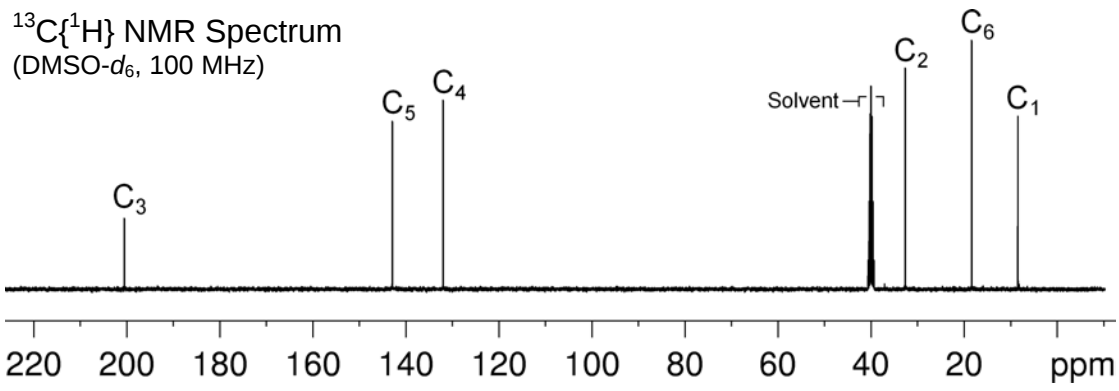
The ^{1}H NMR spectrum has signals at δ 0.96 (H_1), 1.86 (H_6), 2.56 (H_2), 6.11 (H_4) and 6.85 (H_5) ppm.

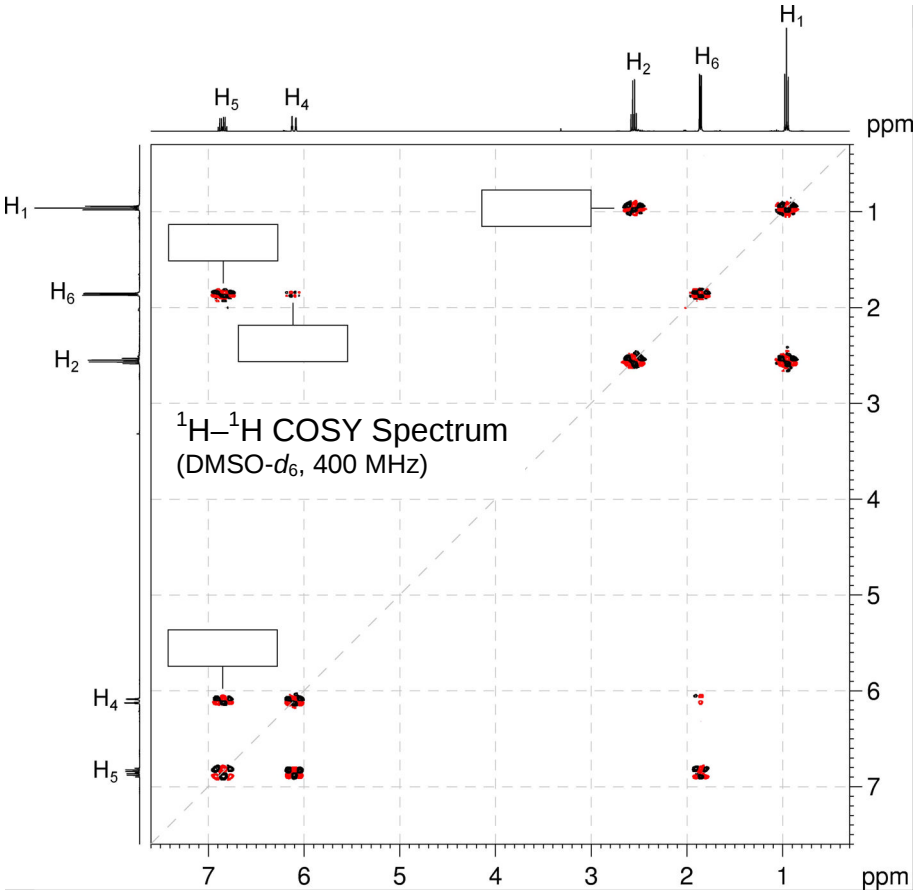
The $^{13}C\{^{1}H\}$ NMR spectrum has signals at δ 8.4 (C_1), 18.4 (C_6), 32.6 (C_2), 131.9 (C_4), 142.8 (C_5) and 200.4 (C_3) ppm.

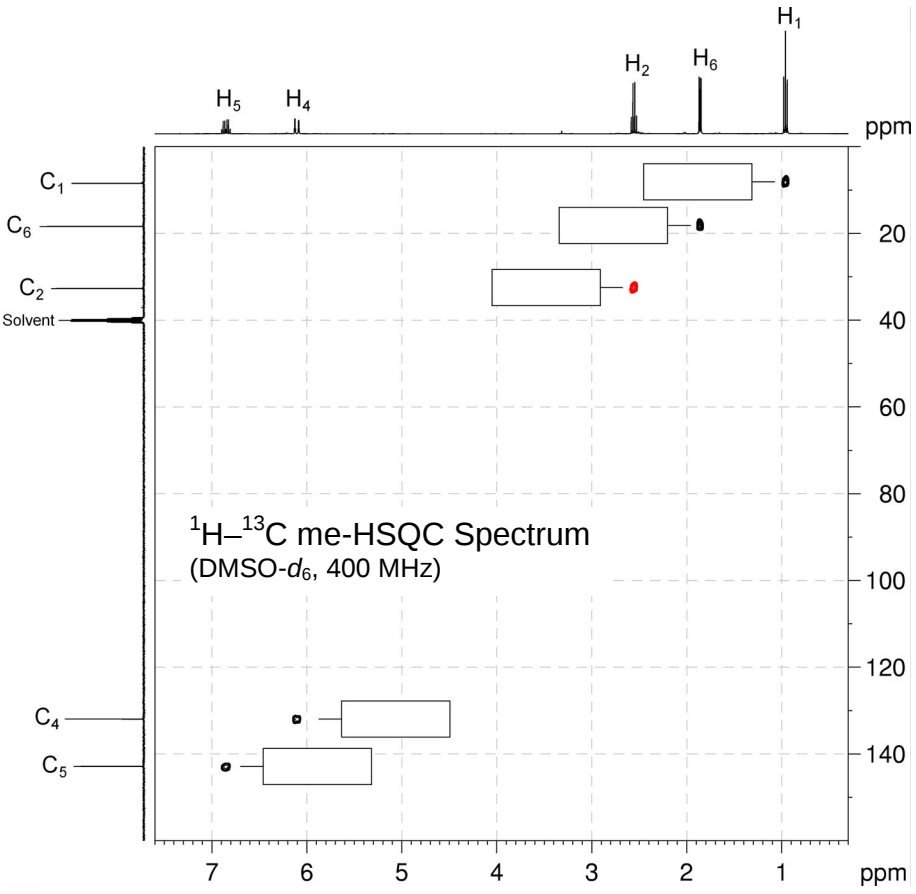
Also given on the following pages are the ^{1}H–^{1}H COSY, ^{1}H–^{13}C me-HSQC, ^{1}H–^{13}C HMBC and ^{1}H–^{1}H NOESY spectra. For each 2D spectrum, indicate which correlation gives rise to each cross-peak by placing an appropriate label in the box provided.








H1
H2
H6
H5
H4
ppm
H1
H6
H2
H4
H5
1H–1H COSY Spectrum
(DMSO-d6, 400 MHz)
1
2
3
4
5
6
7
7
6
5
4
3
2
1
ppm


H1
H2
H6
H5
H4
ppm
C1
C6
C2
Solvent
C4
C5
1H–13C me-HSQC Spectrum
(DMSO-d6, 400 MHz)
20
40
60
80
100
120
140
7
6
5
4
3
2
1
ppm

$^{1}H–^{13}C$ HMBC Spectrum
(DMSO-d_6, 500 MHz)