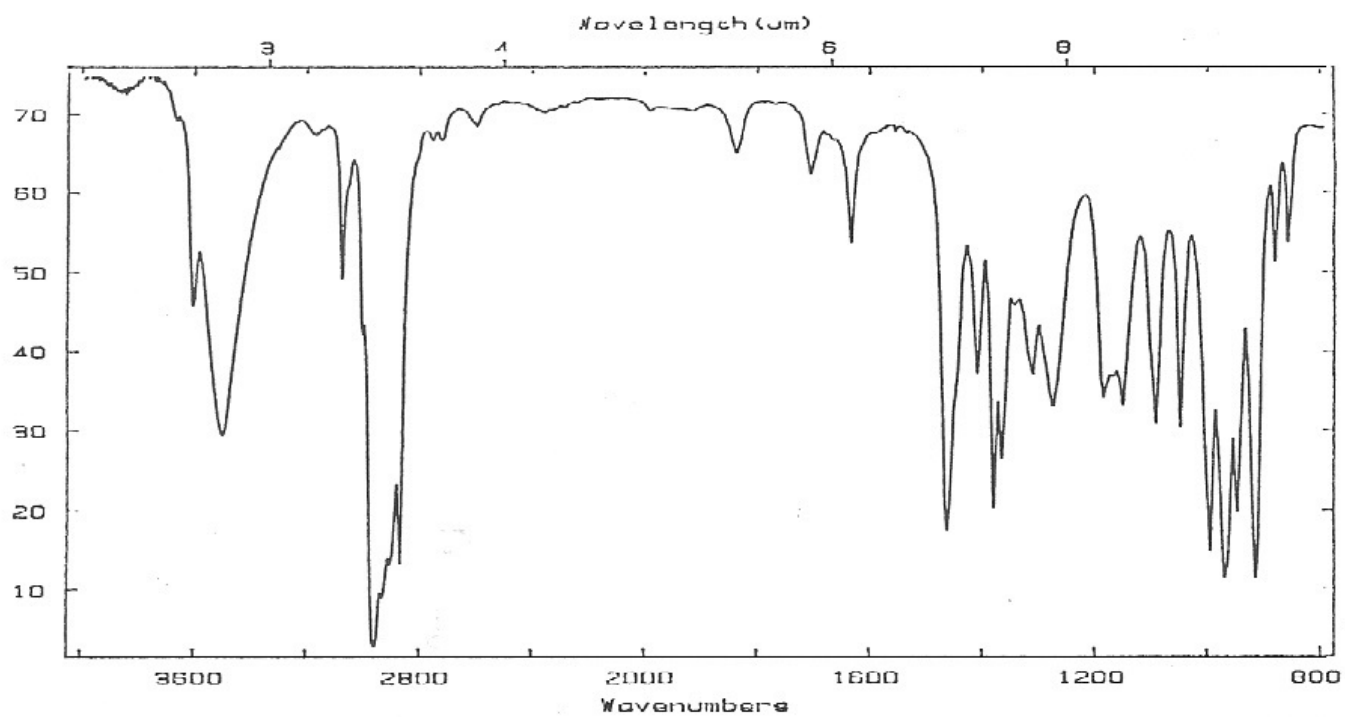
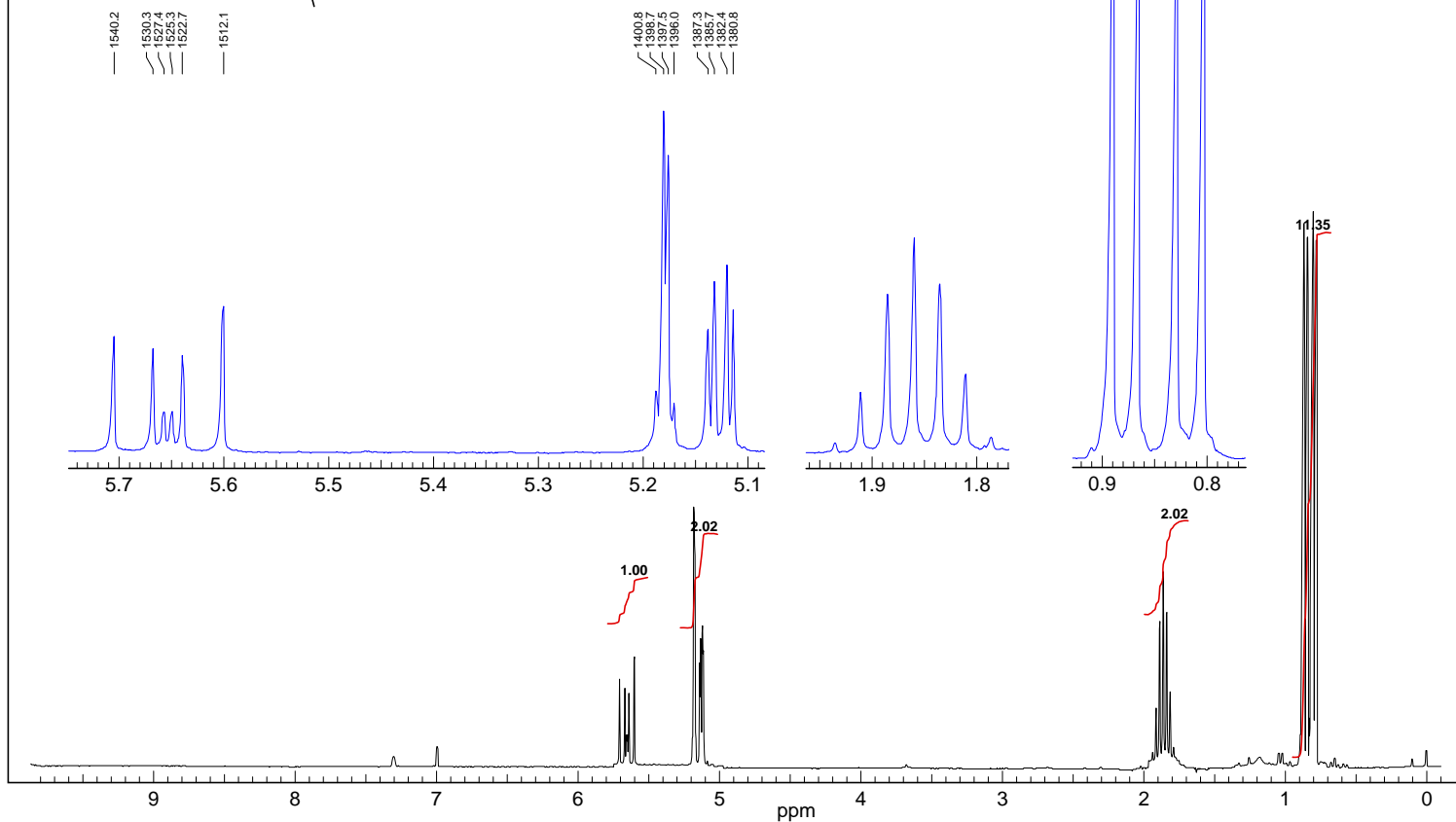
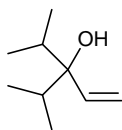


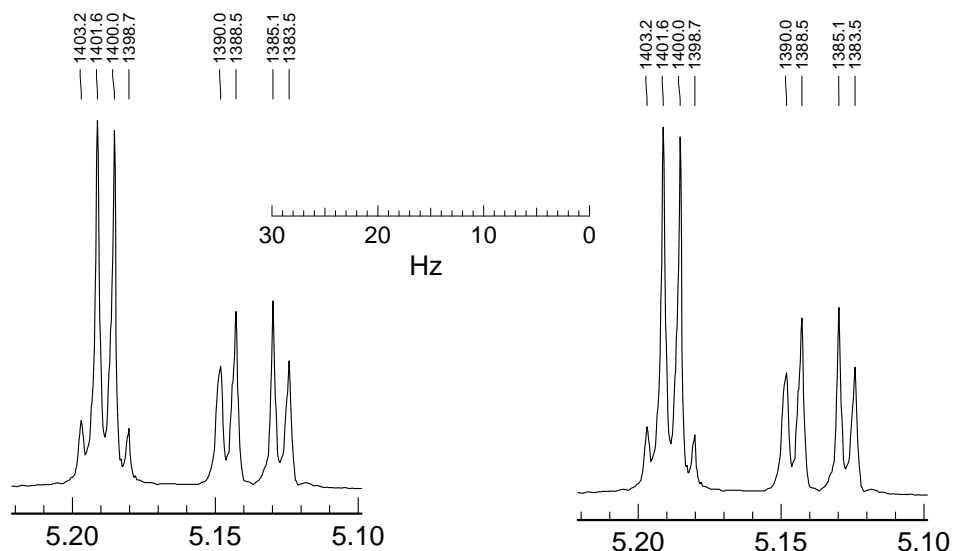
Problem R-06J ($C_9H_{18}O$)270 MHz NMR spectrum in $CDCl_3/C_6D_6$

Source: R. Dykstra/B. Gudmundsson/Reich (digitized hard copy) g

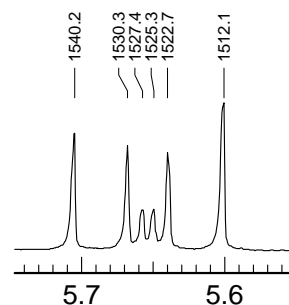


Problem R-06J This problem requires you to analyze the signals at δ 5.1 and 5.7. You are given the structure.

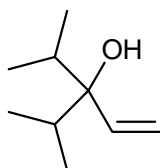
(a) Do qualitative (but correct) solutions on the two reproductions of the multiplet at δ 5.1 below (draw a coupling tree for the two alternative solutions of this multiplet).



(b) Do a quantitative analysis. Use the frequencies given. If more than one solution is possible, show them both, and use appropriate criteria to distinguish the two. Show your work, and tabulate your data in an easily readable form.

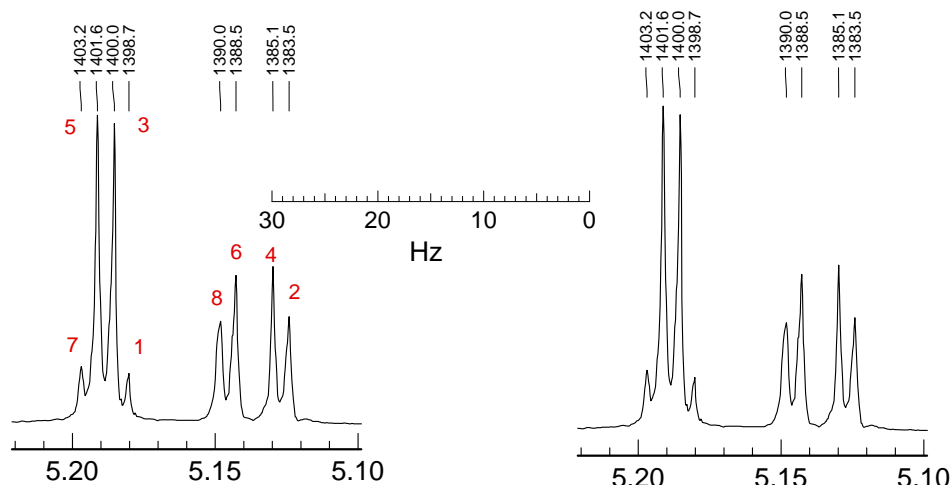


(c) Show J and δ on the structure.

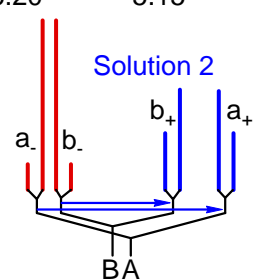
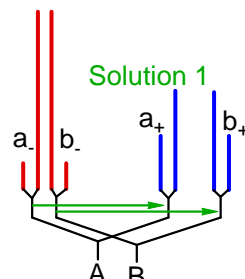


Problem R-06J This problem requires you to analyze the signals at δ 5.1 and 5.7. You are given the structure.

(a) Do qualitative (but correct) solutions on the two reproductions of the multiplet at δ 5.1 below (draw a coupling tree for the two alternative solutions of this multiplet).



The J_{AX} and J_{BX} have the same sign in both Solution 1 and Solution 2



(b) Do a quantitative analysis. Use the frequencies given. If more than one solution is possible, show them both, and use appropriate criteria to distinguish the two. Show your work, and tabulate your data in an easily readable form.

1	1398.7	$c_- = (5+3)/2 = 1400.8$
2	1383.5	$c_+ = (6+4)/2 = 1386.8$
3	1400	
4	1385.1	$\Delta\nu_{ab-} = \nu_- = \sqrt{(7-1)(5-3)} = 2.7$ $c \pm \nu/2 = 1402.1, 1399.5$
5	1401.6	$\Delta\nu_{ab+} = \nu_+ = \sqrt{(8-2)(6-4)} = 4.7$ $c \pm \nu/2 = 1389.2, 1384.4$
6	1388.5	
7	1403.2	
8	1390	

Intensity Calculation

Solution 1

$$\Phi_{1+} = 0.5 \arcsin(J_{AB}/2D_+) = 9.3$$

$$\Phi_{1-} = 0.5 \arcsin(J_{AB}/2D_-) = 12.0$$

$$i_{10} = i_{11} = 0.998$$

$$i_{14} = i_{15} = 0.002$$

Solution 2

$$\Phi_{2+} = \Phi_1 = 9.3$$

$$\Phi_{2-} = 90 - \Phi_{1-} = 78.0$$

$$i_{10} = i_{11} = 0.132$$

$$i_{14} = i_{15} = 0.868$$

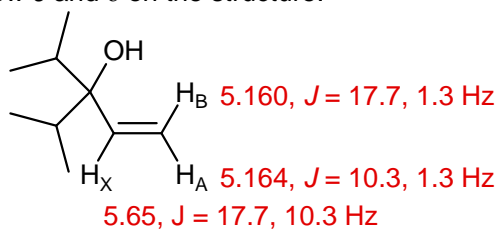
5 Sol1/Sol2 Intensity

9 Data

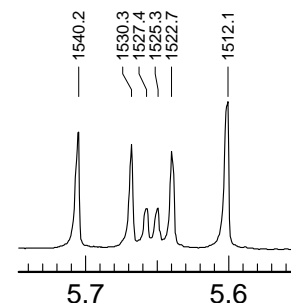
2

Sign of couplings is OK for both Sol. 1 and Sol. 2 (all positive).
Magnitude of couplings is acceptable for both solutions, but better for Sol. 2. Intensity calculation is required to be sure that Sol 2 is correct.

(c) Show J and δ on the structure.



3



NMR Data

Solution 1

$$J_{AB} = 1.3$$

$$J_{AX} = 13.0$$

$$J_{BX} = 15.0$$

$$\nu_A = 1395.6$$

$$\nu_B = 1392.0$$

$$\Delta\nu_{AB} = 3.7$$

$$\delta_A = 5.169$$

$$\delta_B = 5.155$$

Solution 2

$$J_{AB} = 1.3$$

$$J_{AX} = 10.3$$

$$J_{BX} = 17.7$$

$$\nu_A = 1394.3$$

$$\nu_B = 1393.3$$

$$\Delta\nu_{AB} = 1.0$$

$$\delta_A = 5.164$$

$$\delta_B = 5.160$$