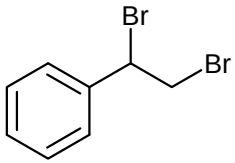
Problem R-10G ($C_8H_8Br_2$)

300 MHz ^{1}H NMR Spectrum in $CDCl_3$

(Source: Wayne Goldenberg/Reich 11/31)

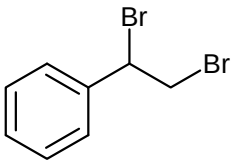


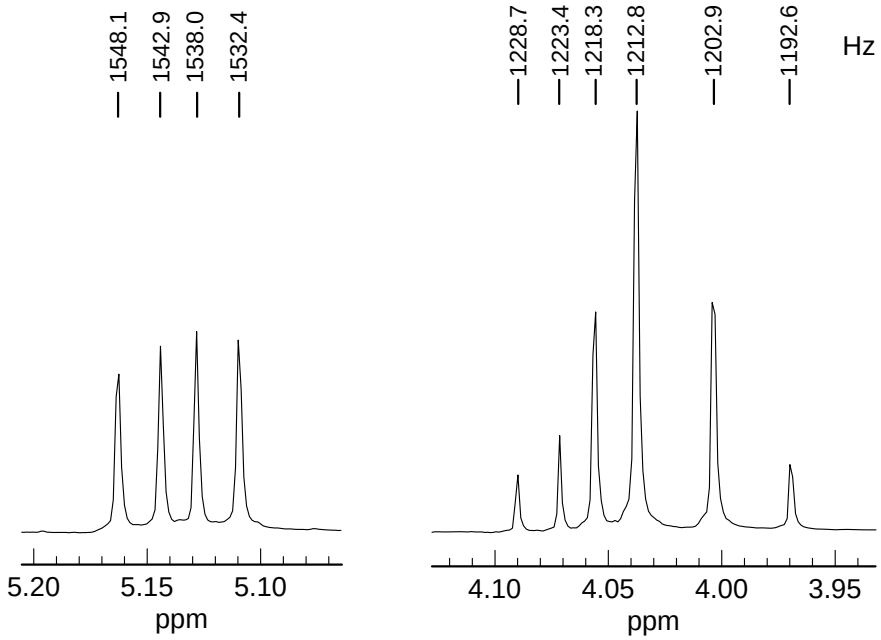
$C_8H_8Br_2$

PLT ex-2-10-11-g.plt

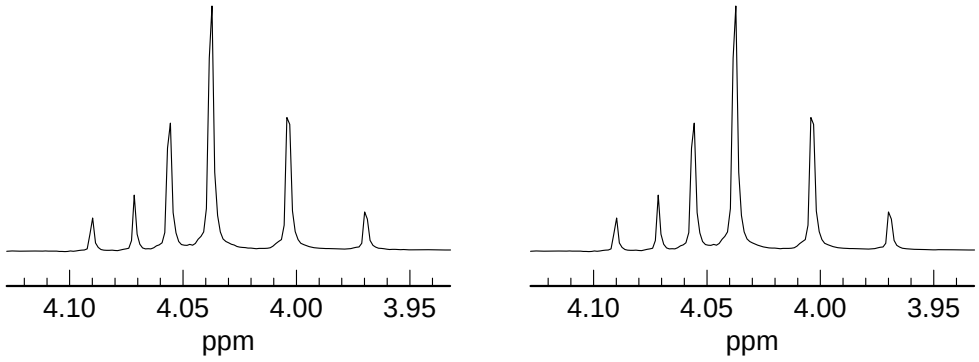
Problem **R-10G** ($C_8H_8Br_2$). This problem requires you to analyze the signals at δ 4.1 and δ 5.2. You are given the structure.

(a) Do a "first order" analysis of the two multiplets shown below. Draw a coupling tree, and estimate couplings. What type of pattern is this?





(b) Do an accurate (quantitative) analysis. Use the frequencies shown above. If more than one solution is possible, show them both, and draw the proper coupling tree on the spectra below. Use appropriate criteria to distinguish the two. Show your work, and tabulate your data in an easily readable form.



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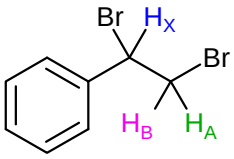

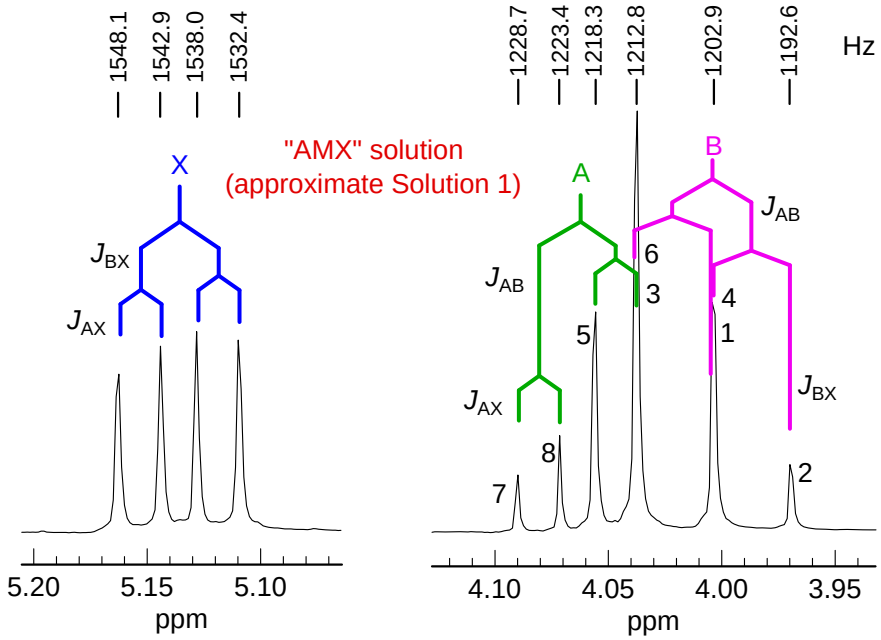

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(b) Do an accurate (quantitative) analysis. Use the frequencies shown above. If more than one solution is possible, show them both, and draw the proper coupling tree on the spectra below. Use appropriate criteria to distinguish the two. Show your work, and tabulate your data in an easily readable form.

1	1202.9
2	1192.6
3	1212.8
4	1202.9
5	1218.3
6	1212.8
7	1228.7
8	1223.4

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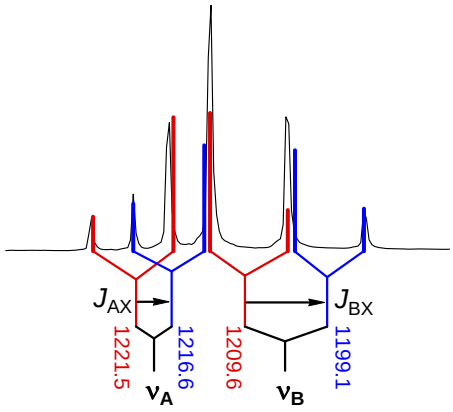
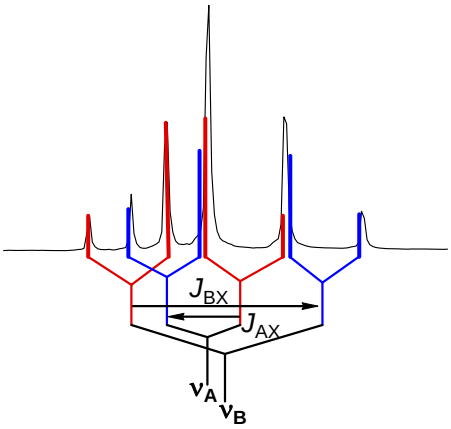
	Solution 1	Solution 2
J_{AB}	9.90 to 10.6	
J_{AX}	+4.93 (-)	-6.99 (+)
J_{BX}	+10.47 (-)	+22.39 (-)
ν_A	1219.04	1213.09
ν_B	1204.36	1210.31
ν_{AB}	14.69	2.77
$i_{10} = i_{11}$	0.995	0.322
δ_A	4.063	4.044
δ_B	4.015	4.034



Solution 1



Solution 2

c- = (5+3)/2 = 1215.55

Δνab- = δ- = sqrt((7-1)(5-3)) = 11.9

c- ± δ-/2 = 1221.5, 1209.6

c+ = (6+4)/2 = 1207.85

Δνab+ = δ+ = sqrt((8-2)(6-4)) = 17.5

c+ ± δ+/2 = 1216.6, 1199.1

Solution 1 is correct:

1. Solution 2 has one negative ^3J, which never happens
2. Intensity calculation fits better for Solution 1