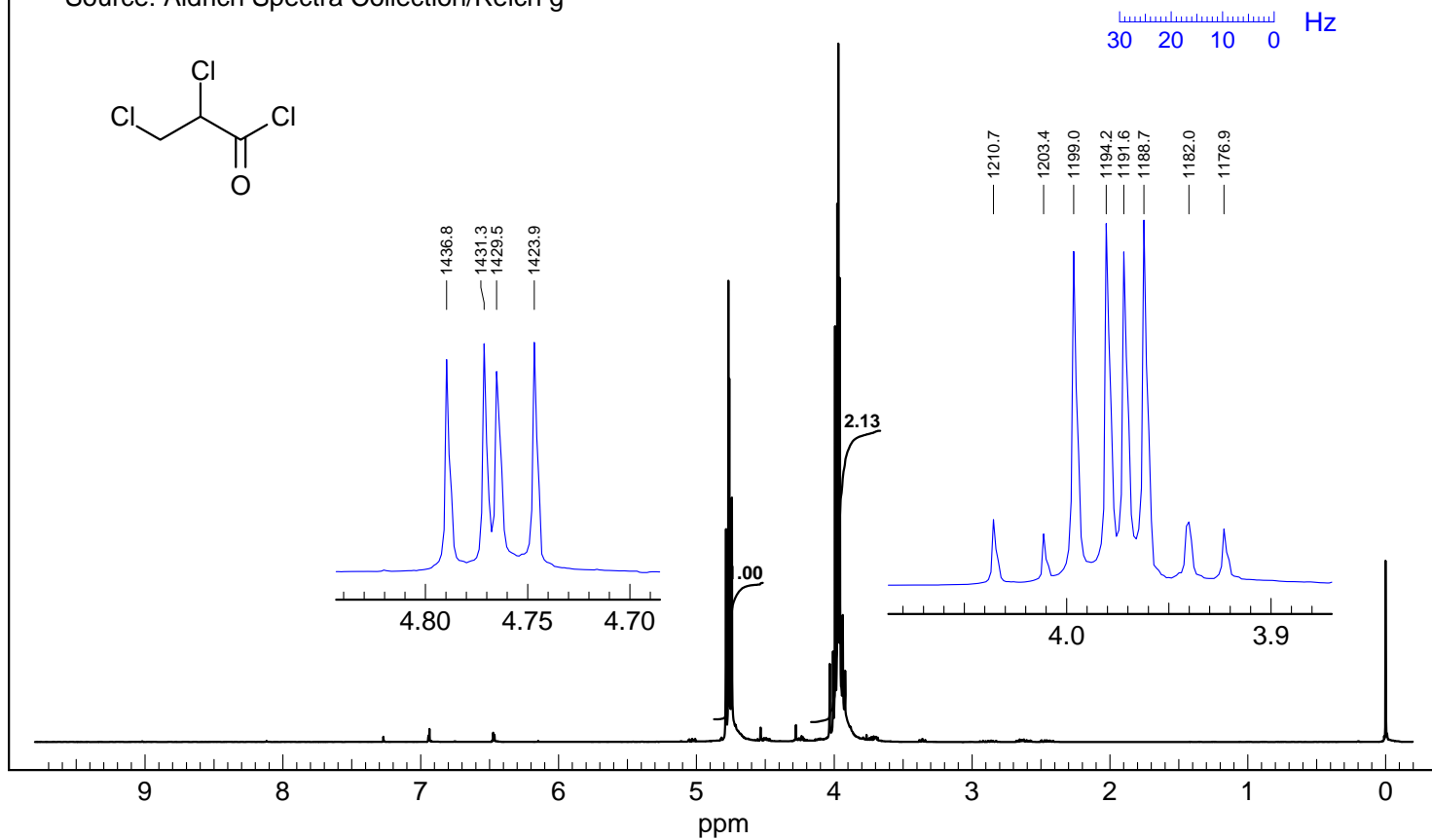
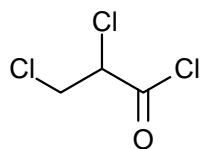


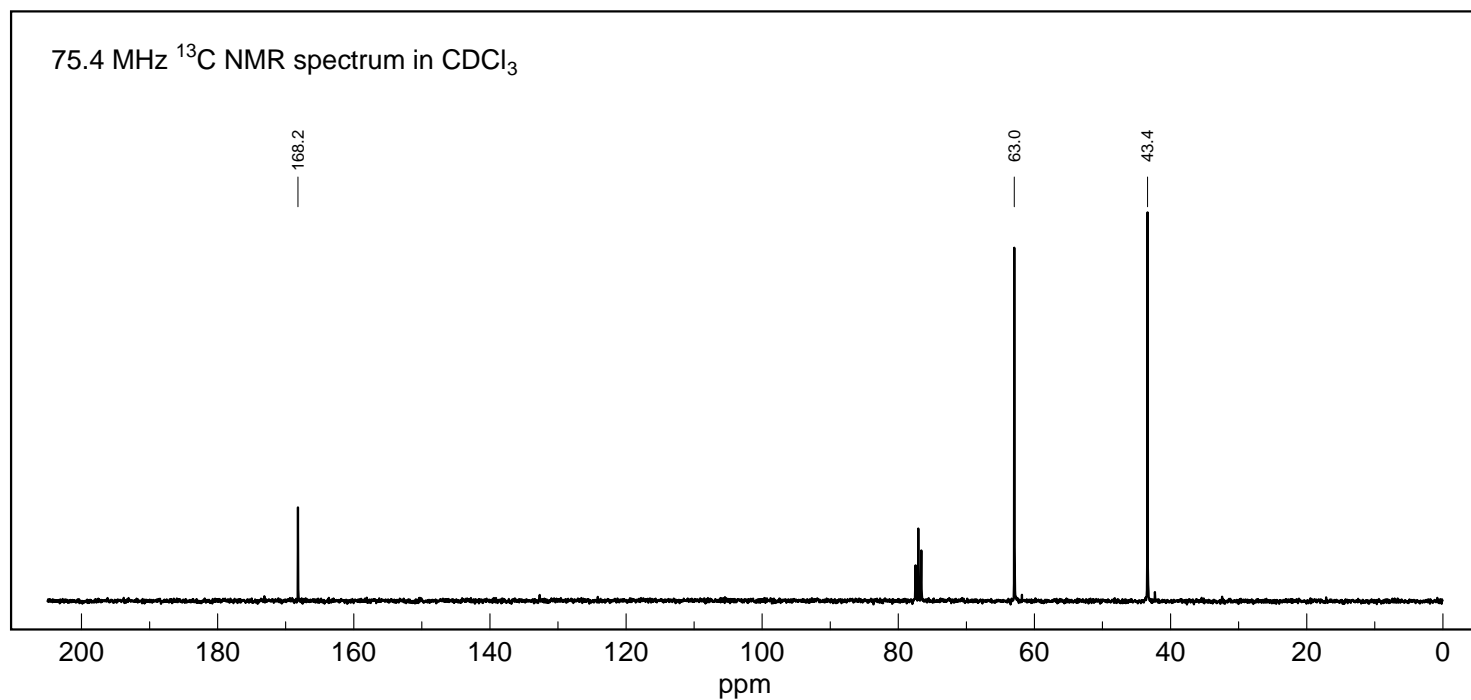
Problem R-12A (C₃H₃Cl₃O)

300 MHz ¹H NMR Spectrum in CDCl₃

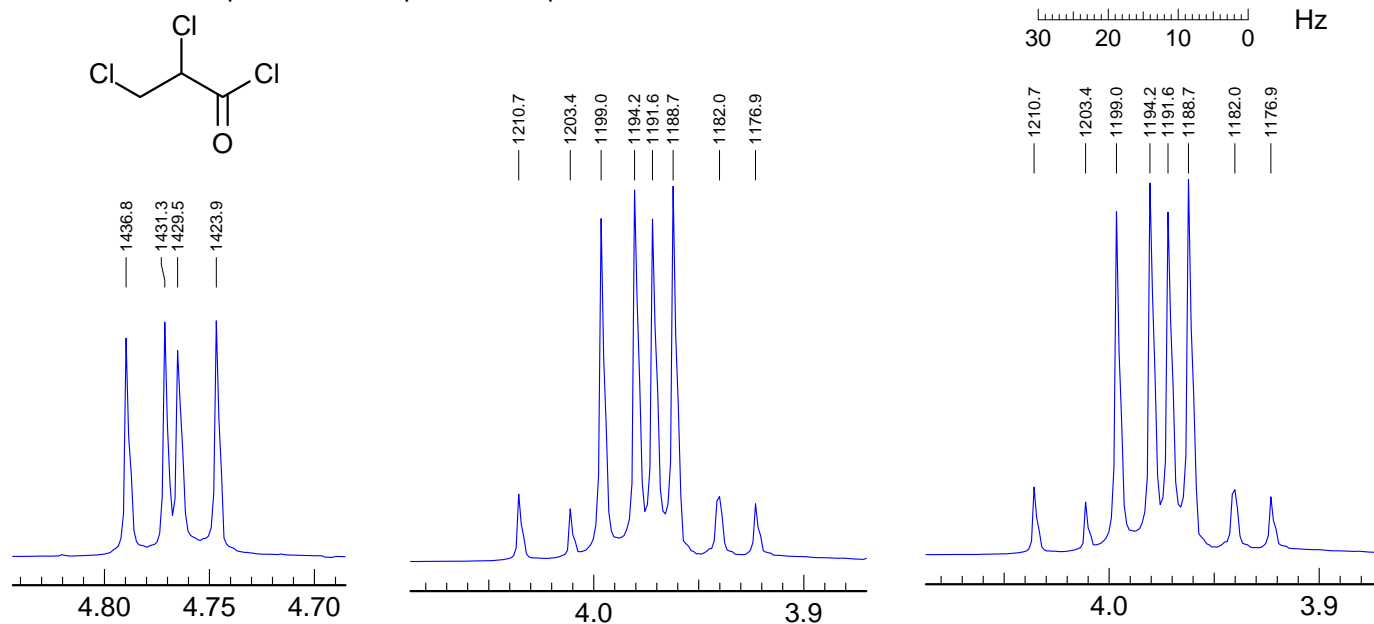
Source: Aldrich Spectra Collection/Reich g



75.4 MHz ¹³C NMR spectrum in CDCl₃



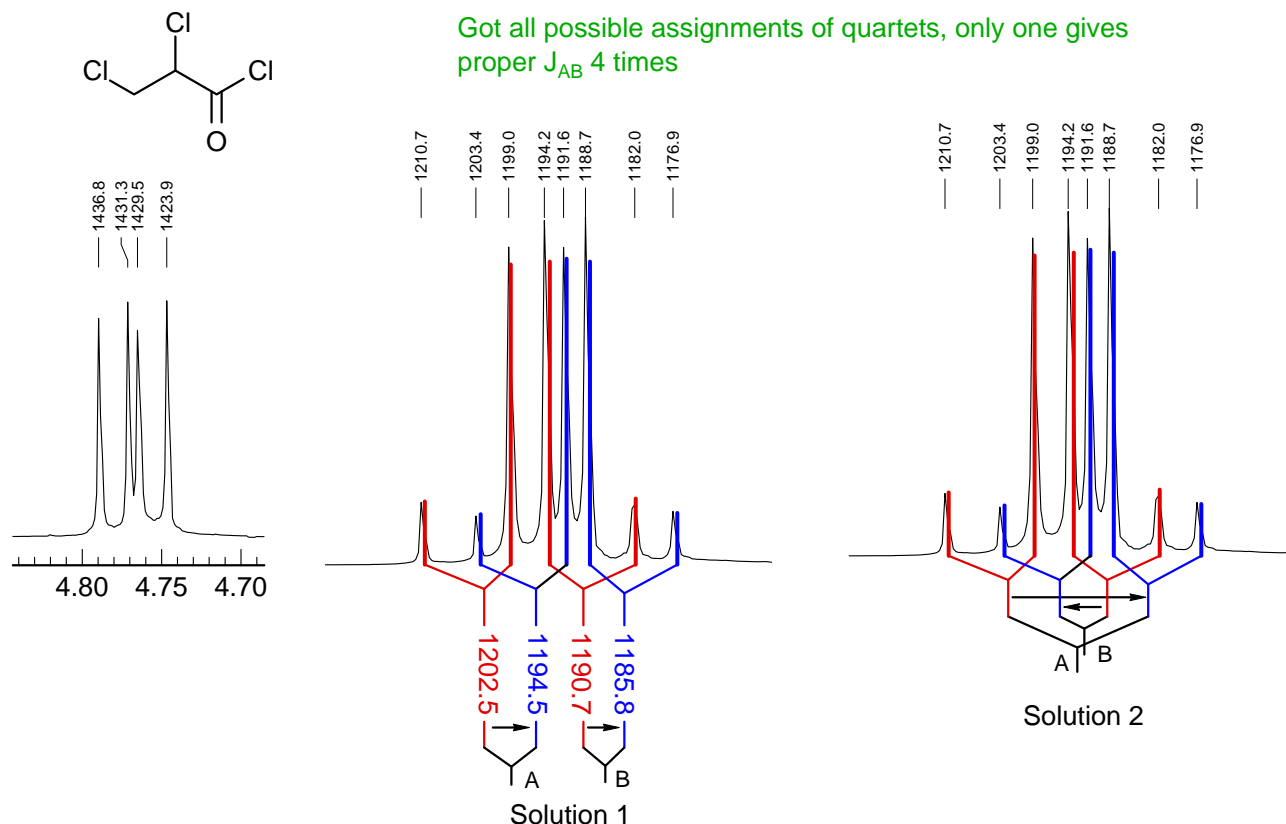
Problem R-12A ($\text{C}_3\text{H}_3\text{Cl}_3\text{O}$). The complete 300 MHz ^1H NMR spectrum of R-12A is shown below. Do an accurate calculation and determine couplings and chemical shifts, and **tabulate your results in an easily readable format**. If there are two solutions, report them both, and draw coupling trees on the spectra. For your convenience two copies of the AB part of the spectrum are shown.



(a) Show a coupling tree, and do a mathematically accurate analysis of this spectrum. If there are two solutions, report them both. Show your work, and tabulate your data in an easily readable form.

(b) If you are proposing two solutions, suggest at least one criterion which allows you to identify the correct one.

Problem R-12A ($C_3H_3Cl_3O$). The complete 300 MHz 1H NMR spectrum of R-12A is shown below.

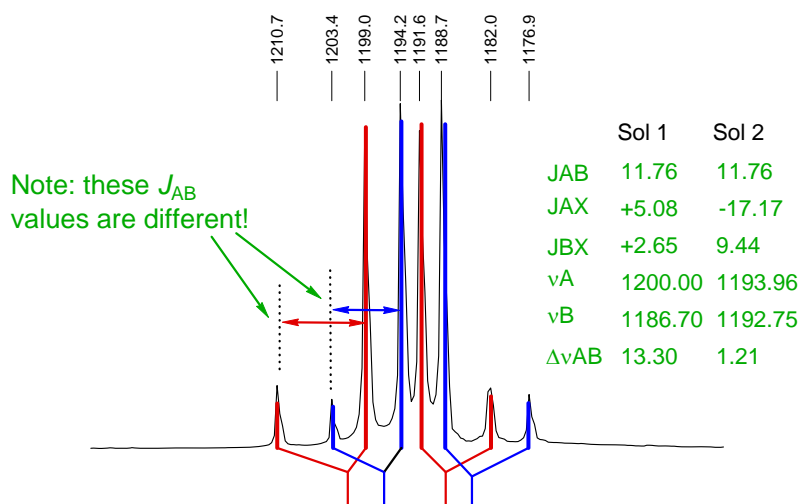


(a) Show a coupling tree, and do a mathematically accurate analysis of this spectrum. If there are two solutions, report them both. Show your work, and tabulate your data in an easily readable form.

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	Sol. 1	Sol. 2	
J_{AB}	11.8	11.8	or
J_{AX}	7.9	-16.7	+16.7
J_{BX}	5.0	+3.8	-3.8
ν_A	1198.5	1194.1	
δ_A	3.995	3.980	
ν_B	1188.2	1192.6	
Δ_B	3.96	3.98	
$\Delta\nu_{AB}$	10.3	1.5	
$i_{10} = i_{11}$	0.996	0.580	
$i_{14} = i_{15}$	0.004	0.420	

Most common wrong assignment of lines



(b) If you are proposing two solutions, suggest at least one criterion which allows you to identify the correct one.

3 Given the structure, the signs of J_{AX} and J_{BX} must be both be positive, so Sol. 1 is correct. Can also use calculated intensities, which are very different for Sol 1 and Sol 2. Size of the couplings is not a very solid criterion in this case.