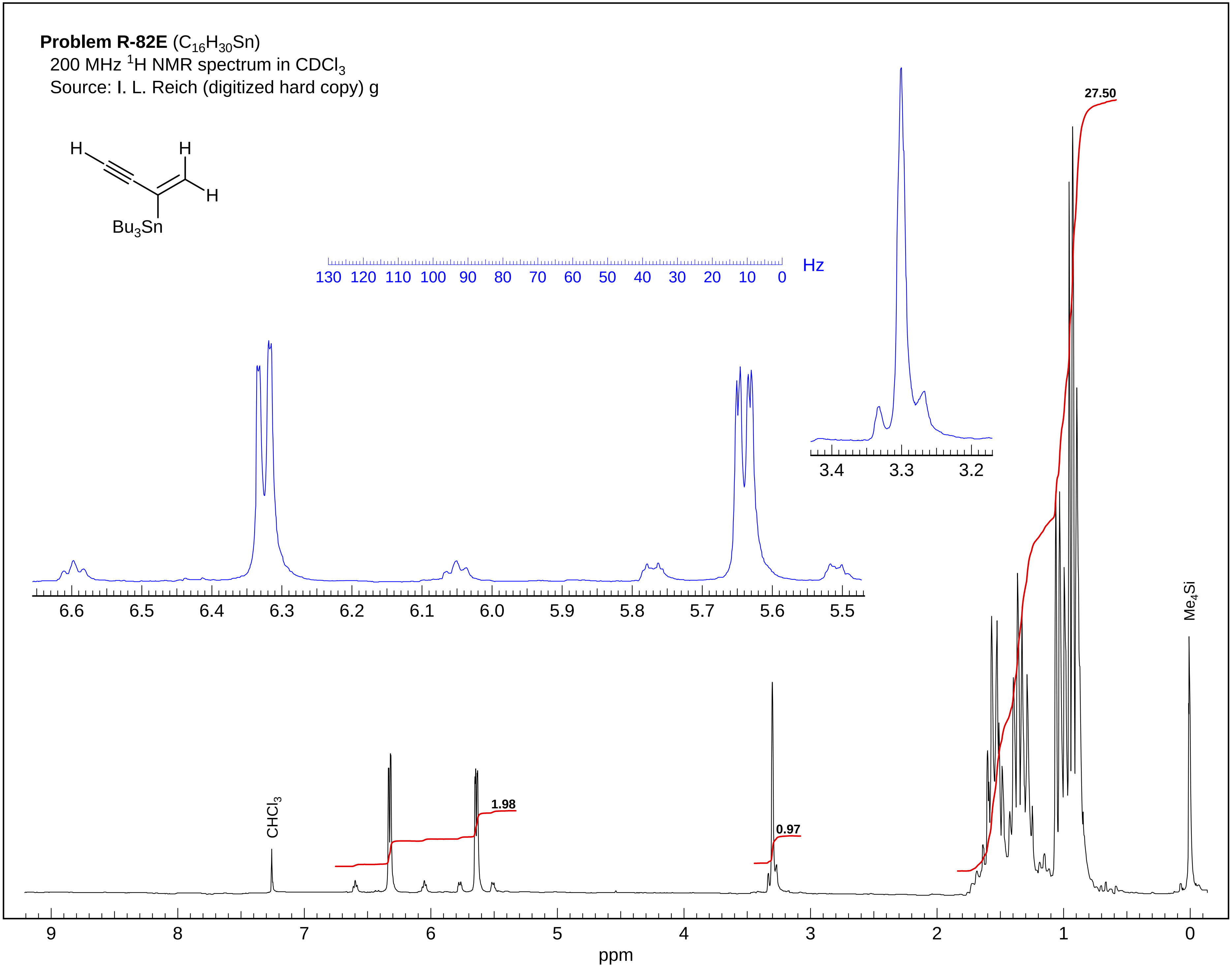
Problem R-82E ($C_{16}H_{30}Sn$)
200 MHz ^{1}H NMR spectrum in $CDCl_3$
Source: I. L. Reich (digitized hard copy) g



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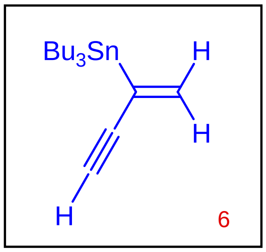
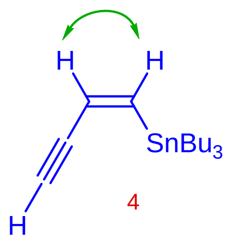
Problem R-82E ($C_{16}H_{30}Sn$). Consider carefully the ^{1}H NMR spectrum of R-82E shown on the next page (the compound contains a tri-n-butyltin group, tin is tetravalent).

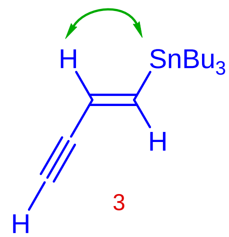
(a) DBE?__3__ What is the structure of R-82E?


6

4 Hz is too small


4

4 Hz is definitely too small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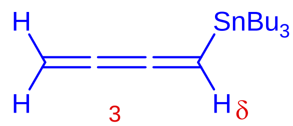
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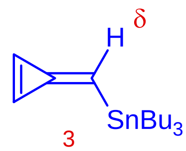
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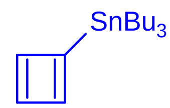


(b) Explain the origin and shape of the multiplets at δ 6.05 and 6.6.

Sn has two main spin 1/2 isotopes (the third one is not abundant enough to detect in these spectra:

^{119}Sn	8.7%	37.28
^{117}Sn	7.1%	35.63
^{115}Sn	0.34%	32.17

Thus each peak will have two pairs of satellites, one set due to ^{117}Sn and one to ^{119}Sn

(c) Determine (approximately) all coupling constants that can be obtained from the spectrum. Identify them in the form $^4J_{XY}$ = Z Hz. Label your structure so that it is clear which atom you are referring to.

^3J (H^A-^{117}Sn) = 107 Hz

^3J (H^B-^{117}Sn) = 52 Hz

^3J (H^A-^{119}Sn) = 113 Hz

^3J (H^B-^{119}Sn) = 54 Hz

$^5J_{AC}$ ca 0.5 Hz

$^2J_{AB}$ = 4 Hz

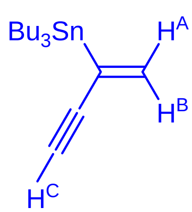
$^5J_{BC}$ = 1 Hz

$^2J_{BA}$ = 4 Hz

^4J(H^C-Sn) = 14 Hz

$$\frac{\gamma\,(^{119}\text{Sn})}{\gamma\,(^{117}\text{Sn})} = \frac{37.28}{35.63} = 1.046$$

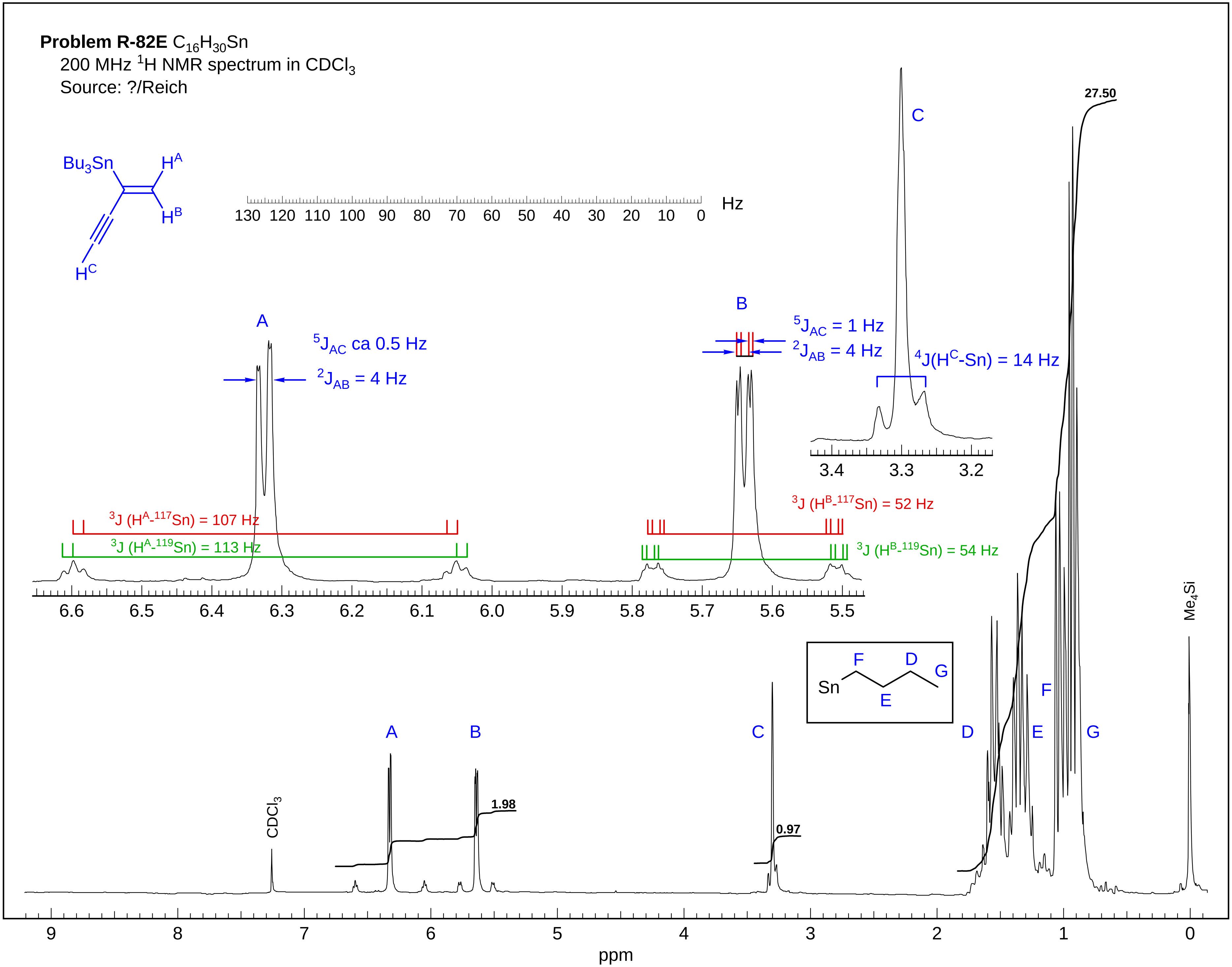
Thus get two sets of satellites, differing by ca 4% in J



Problem R-82E $C_{16}H_{30}Sn$

200 MHz ^{1}H NMR spectrum in $CDCl_3$

Source: ?/Reich



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