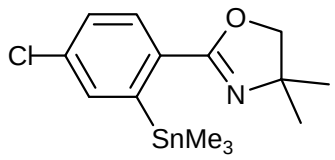
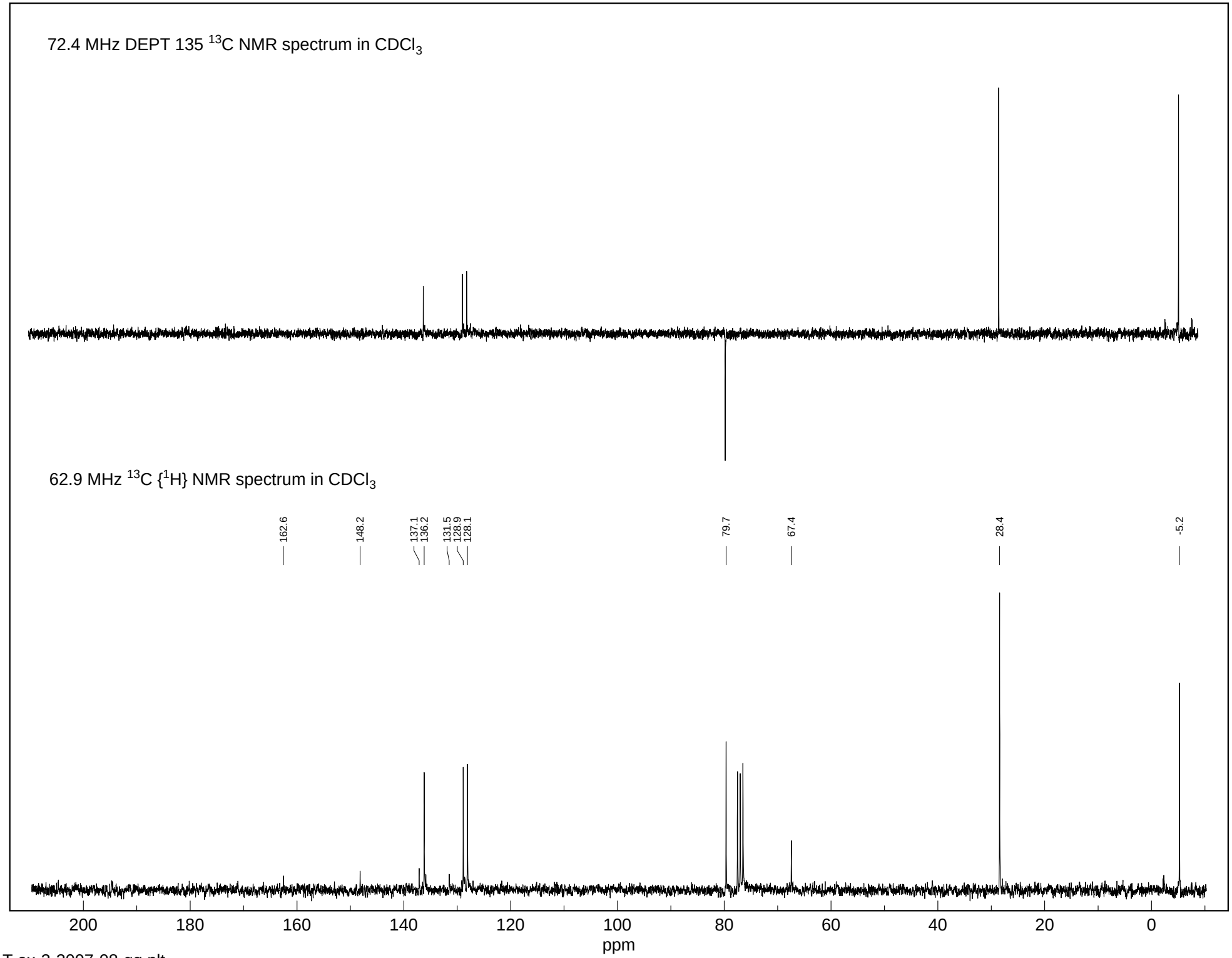
Problem R-07L ($C_{14}H_{20}ClNOSn$)
300.1 MHz ^{1}H NMR Spectrum in $CDCl_3$.
Source: Kevin Jantzi (Reich) g



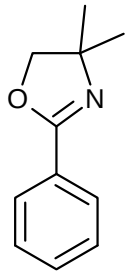
PLT ex-3-2007-08-gq.plt



PLT ex-3-2007-08-gq.plt

Problem R-07L ($C_{14}H_{20}ClNOSn$). You are given a partial structure of a trisubstituted benzene and asked to determine the complete structure.

(a) Do a complete analysis of the 300 MHz ^{1}H NMR spectrum of R-07L, determine the structure, and determine all chemical shifts and coupling constants. Complete the structure below, and write the chemical shifts on it. Report all couplings in the form $^{n}J_{HX}$ = 00 Hz (specify nucleus, if appropriate).

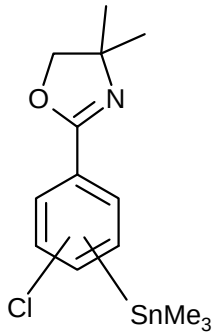


(b) Briefly describe how you made the assignment of the substitution pattern

Problem R-07L ($C_{14}H_{20}ClNOSn$)

00.1 MHz ^{1}H NMR Spectrum in $CDCl_3$.

Source: Kevin Jantzi (Reich) g



PLT ex-3-2007-08-gq.plt

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Problem R-07L ($C_{14}H_{20}ClNOSn$). You are given a partial structure of a trisubstituted benzene and asked to determine the complete structure.

(a) Do a complete analysis of the 300 MHz ^1H NMR spectrum of R-07L, determine the structure, and determine all chemical shifts and coupling constants. Complete the structure below, and write the chemical shifts on it. Report all couplings in the form $^nJ_{HX}$ = 00 Hz (specify nucleus, if appropriate).

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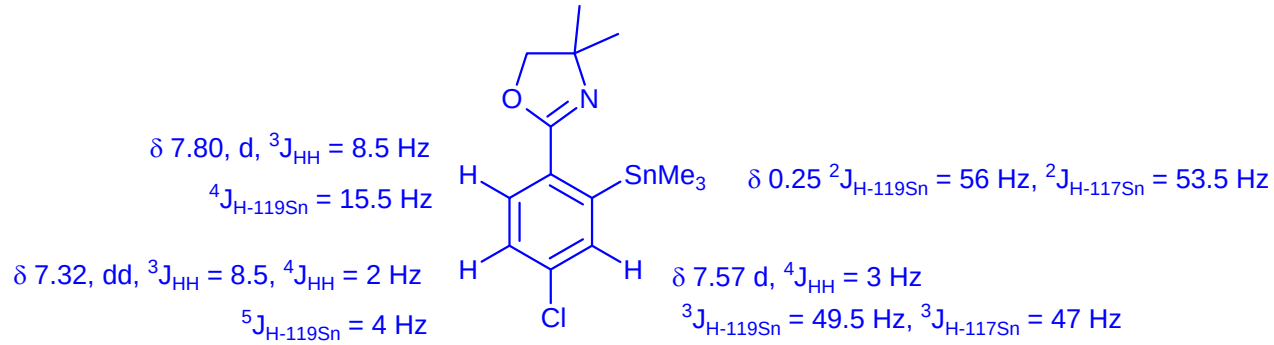

Assume: $^3J_{HSn}$ (ortho) > $^4J_{HSn}$ (meta) > $^5J_{HSn}$ (para)

(b) Briefly describe how you made the assignment of the substitution pattern

The proton NMR couplings require a 1,2,4-substitution pattern. There are 6 possible isomers:

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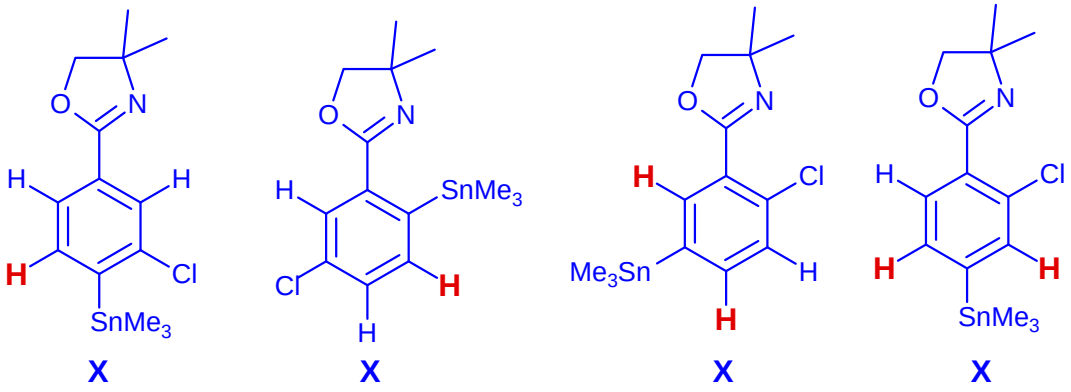
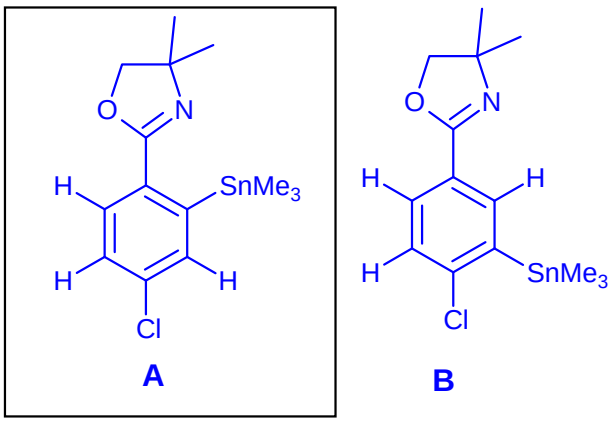


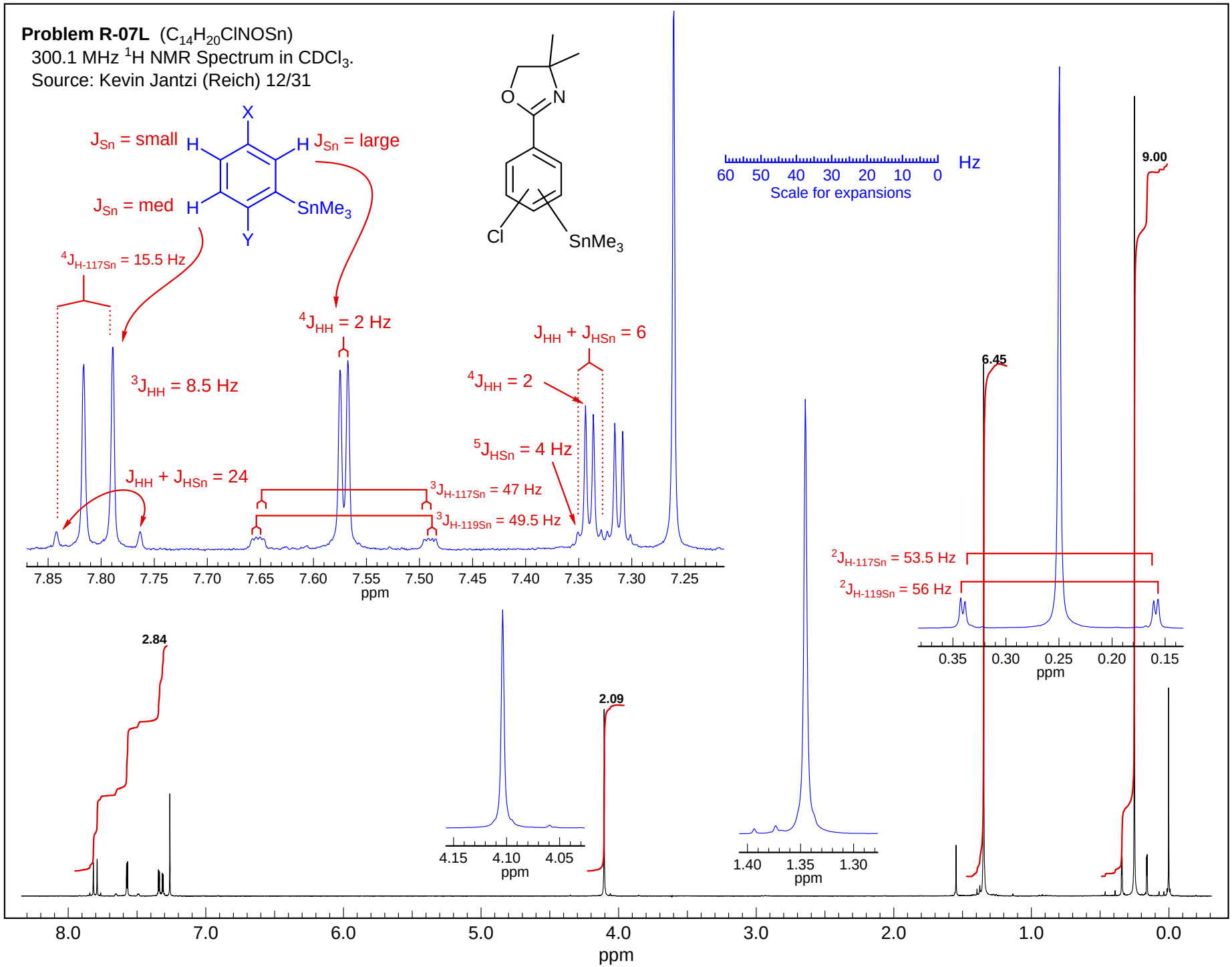
The proton which is ortho to Sn has NO ortho H's

Me_3Sn group does NOT have 2 ortho hydrogens (only one H has large H-Sn coupling)



These are the two possible structures that fit J_{HH} and J_{HSn}. Since oxazoline group should have ortho chemical shifts like a carbonyl group, structure A is preferred, because there is only one downfield proton (δ 7.8), whereas B would have 2

Split about evenly between A and B



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