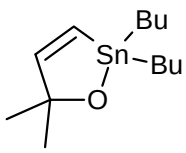
Problem R-08M $C_{13}H_{26}OSn$

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

Source: Ken Yelm/Reich (digitized hard copy) g



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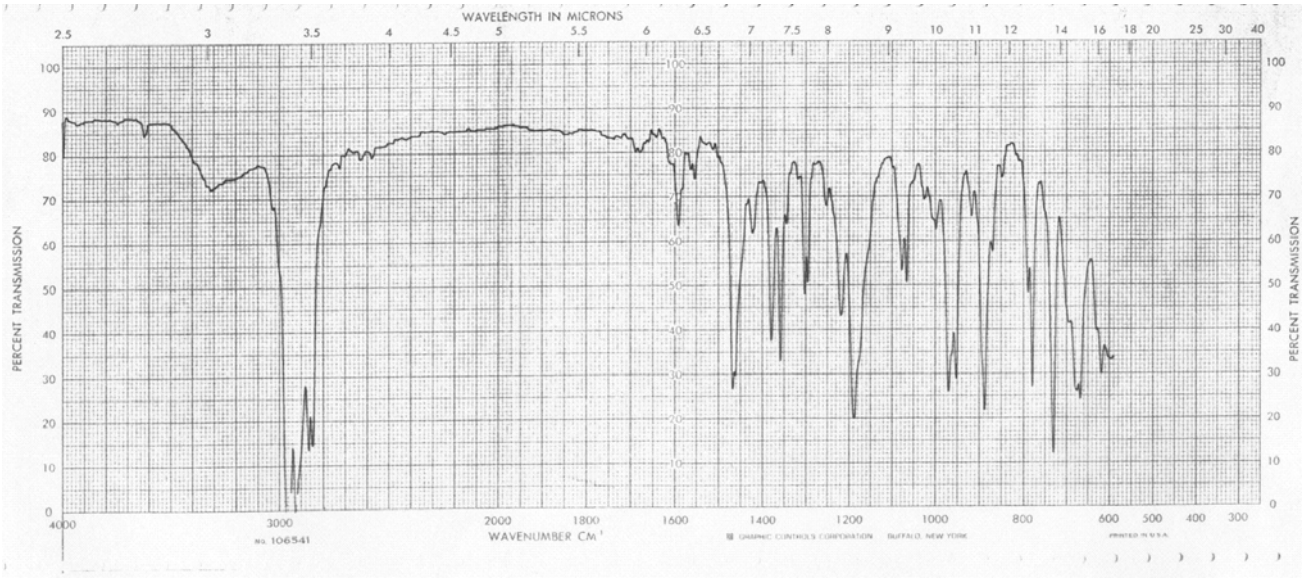
Problem R-08M ($C_{13}H_{26}OSn$) You are asked to determine the structure and interpret the ^1H NMR spectrum. The compound contains two n-butyl groups, and is a Sn(IV) compound.

(a) DBE___ (b) Interpret the IR spectrum.



(b) Show any part structures you have identified from consideration of the NMR and IR spectra, and give the spectral data you used to make the assignment. Draw a structure for **R-08M**.

Structure:

(c) Analyze completely the NMR pattern in the expanded region between δ 5.8 and 7.6. Report all couplings in the standard format ($^nJ_{XY}$ = 112 Hz).

(d) To check your answer, find a model compound or estimate the chemical shifts for the protons at δ 6-7. Show your model or parameters.

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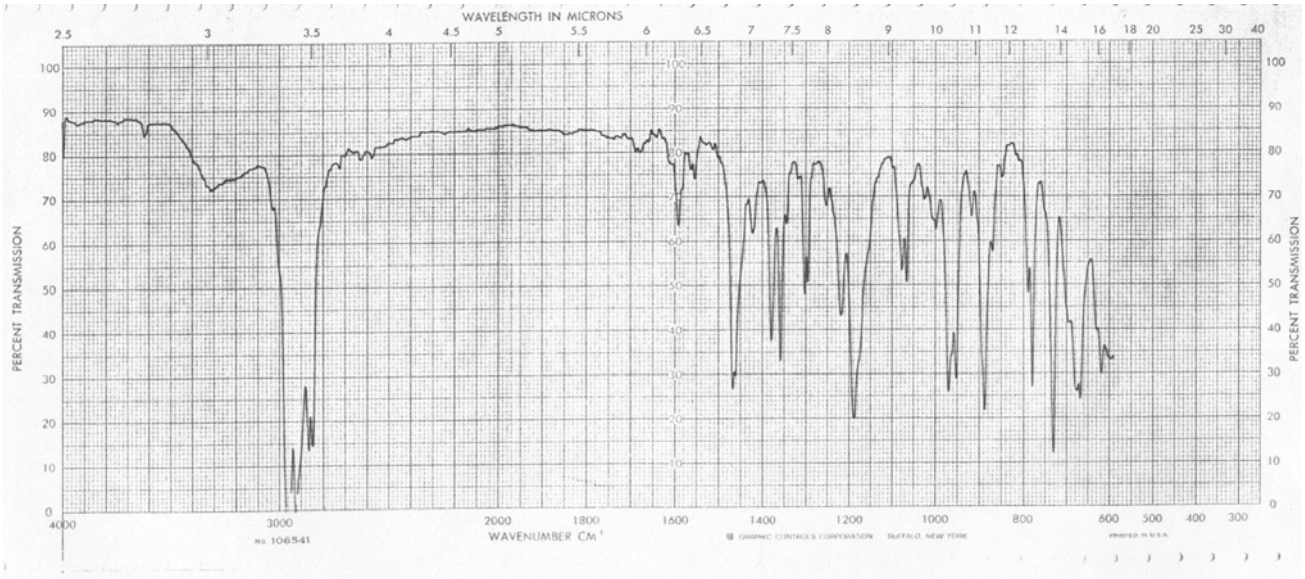
(a) DBE 2 (b) Interpret the IR spectrum.

1

-No carbonyl (nothing between 1550-1800 cm^{-1})
-no triple bond or cumulene (allene) visible around 2000 cm^{-1}
3 -Very likely no OH (peak at 3300 cm^{-1} is too small to be OH)



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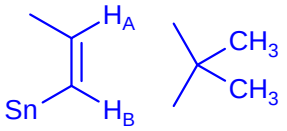
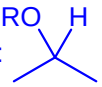


cis double bond

From chemical shifts of butyl, they must both be equivalent, and on Sn ($SnBu_2$), since most downfield signal is a quartet, and thus not the R-CH_2-Pr signal.

no: 

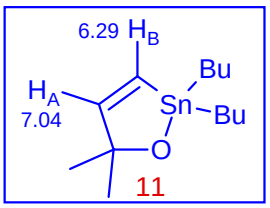
11

Structure:

(c) Analyze completely the NMR pattern in the expanded region between δ 5.8 and 7.6. Report all couplings in the standard format ($^nJ_{XY}$ = 112 Hz).

Calc H_A:
5.25 (Base)
0.64 (g-CO)
0.90 (t-Sn)
6.80 Δδ 0.24

Calc H_B:
5.25 (BASE)
-0.02 (t-CO)
1.21 (g-Sn)
6.44 Δδ 0.15



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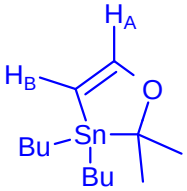
Correct

9

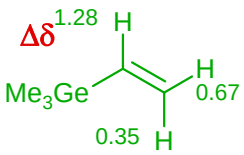
Calc H_A:
5.25 (Base)
1.22 (α-O)
0.90 (t-Sn)
7.37 Δδ 0.31

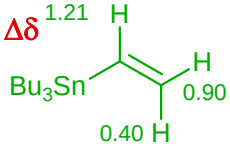
Calc H_B:
5.25 (BASE)
-1.21 (t-O)
1.21 (g-Ge)
5.25 **Δδ 1.04**



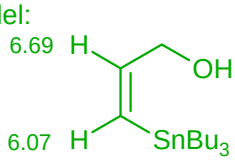
Chemical shift of H_B is off a lot for this isomer

	Correct	Wrong
$^3J_{HA-119Sn}$ = 178.0 Hz		195
$^3J_{HA-117Sn}$ = 170.0 Hz		175
$^2J_{HB-119Sn}$ = 189.0 Hz		184
$^2J_{HB-117Sn}$ = 181.0 Hz		164
$^3J_{HB-HA}$ = 10.0 Hz		





Model:



Common Errors:
- Wrong upper half of downfield multiplet (-4)
- J = 1/2 J (-4)
- wrong coupling tree (-3)

3

(d) To check your answer, find a model compound or estimate the chemical shifts for the protons at δ 6-7. Show your model or parameters.

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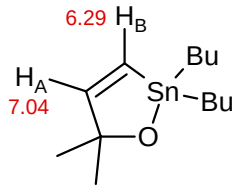

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