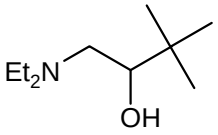
Problem R-07J ($C_{10}H_{23}NO$)
300 MHz ^1H NMR spectrum in $CDCl_3$
Source: Olafs Daugulis/Vedejs (od2177001) g



ABX, ABX_3

PLT ex-2-2007-08-gq.plt

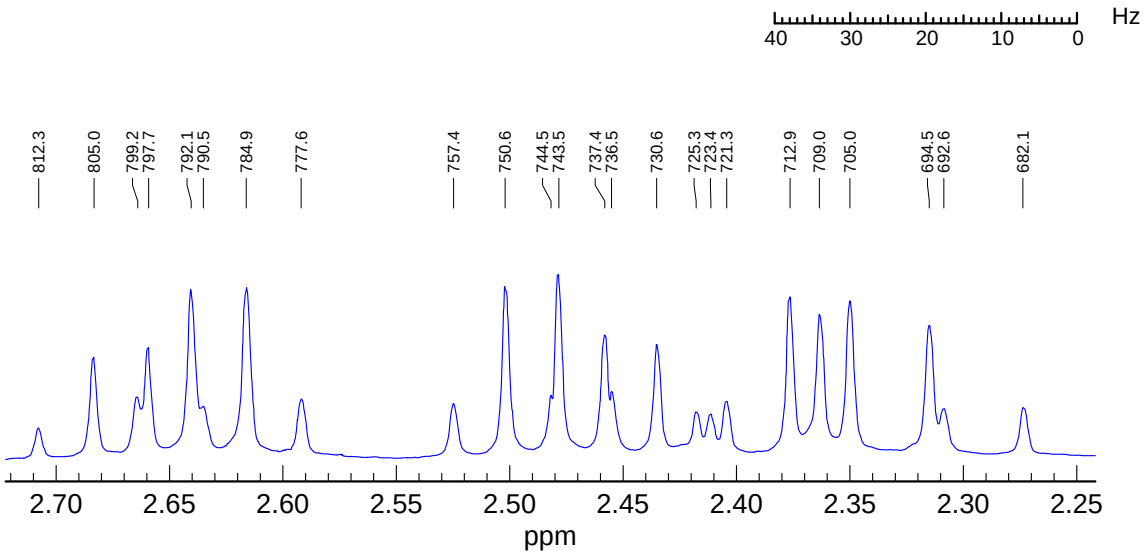
Problem R-07J ($C_{10}H_{23}NO$) Interpret the ^1H NMR spectrum and determine the structure of **R-07J**.

(a) DBE:_____

(b) The singlet at δ 4.05 disappears on addition of D_2O. What does this tell you about the structure?

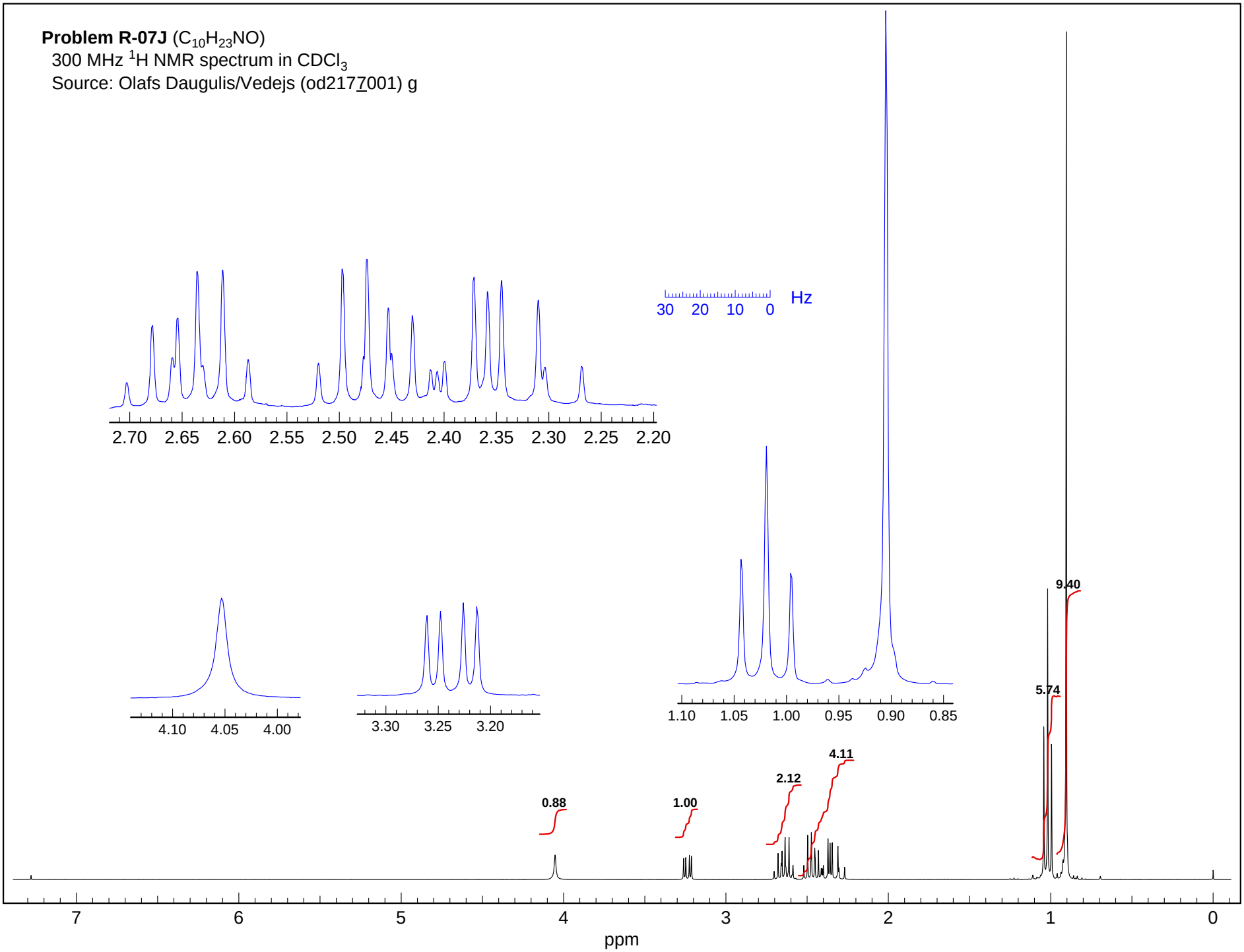
(c) Suggest part structures for the signals at δ 0.9 and δ 1.0.

(d) Do a complete interpretation of the 6-proton multiplet between δ 2.2 and δ 2.7. Measure all couplings and chemical shifts, report them in the standard format, and assign them to the structure reported in part (e). Draw a "coupling tree" on the spectrum. You may use first order analysis if applicable.



(e) Draw the structure of **R-07J** below. If more than one structure fits the data, draw them, but circle your best choice.

(f) Are there features of the NMR spectrum which provide some hints as to the conformation of **R-07J**?



PLT ex-2-2007-08-gq.plt

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Problem R-07J ($C_{10}H_{23}NO$) Interpret the ^1H NMR spectrum and determine the structure of **R-07J**.

1 (a) DBE: 0

(b) The singlet at δ 4.05 disappears on addition of D_2O. What does this tell you about the structure?

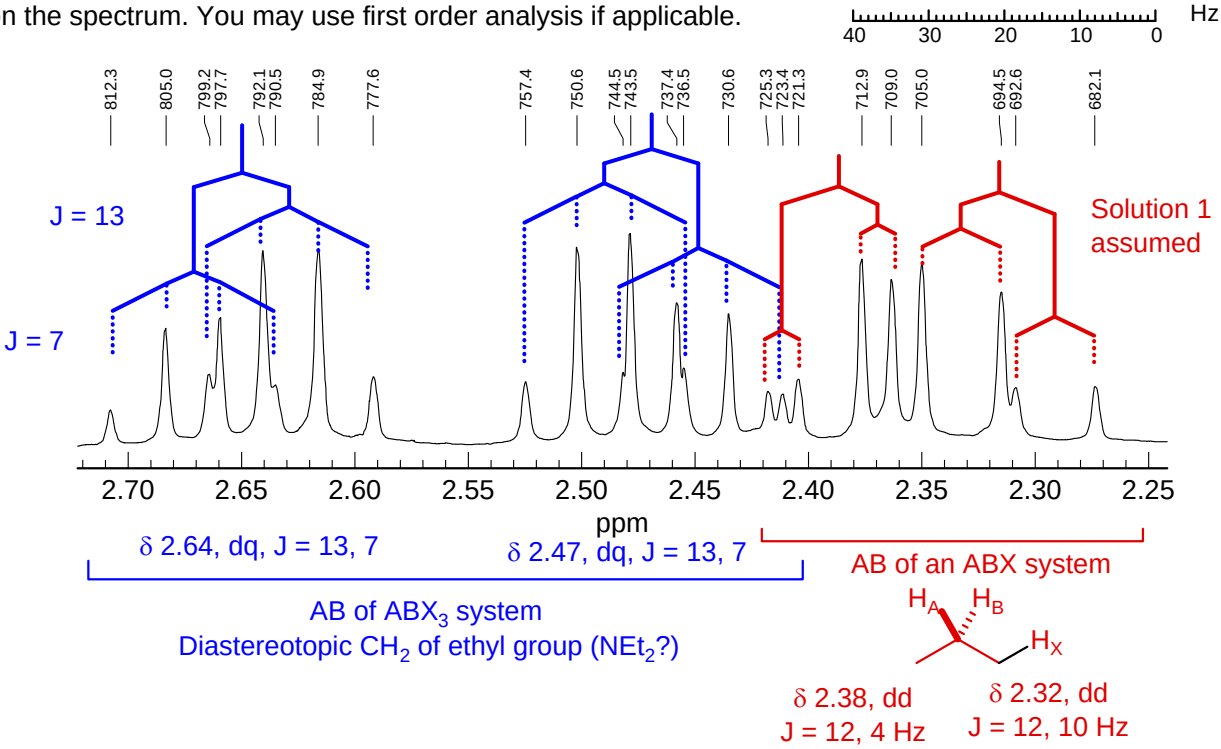
2 This is probably an OH (or possibly NH) signal

(c) Suggest part structures for the signals at δ 0.9 and δ 1.0.

The 9-proton singlet at δ 0.90 is very likely a t-butyl group $-C(CH_3)_3$

4 The 6-proton triplet is probably the CH_3 of a double ethyl group (also possible: diastereotopic $CH(CH_3)_2$ group with accidental coincidence of middle peaks.

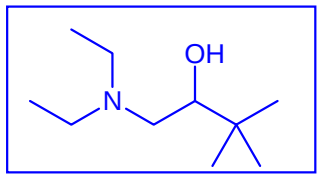
(d) Do a complete interpretation of the 6-proton multiplet between δ 2.2 and δ 2.7. Measure all couplings and chemical shifts, report them in the standard format, and assign them to the structure reported in part (e). Draw a "coupling tree" on the spectrum. You may use first order analysis if applicable.



10

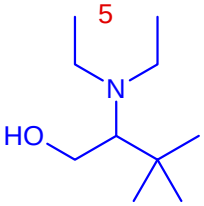
(e) Draw the structure of **R-07J** below. If more than one structure fits the data, draw them, but circle your best choice.

7



δ calc CH 4.0 (obs 3.2)
δ calc CH_2 2.8 (obs 2.4)
Σ Δδ: 1.2

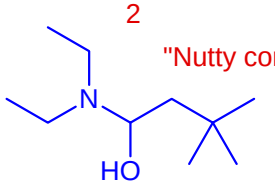
5



δ calc CH 2.9 (obs 3.2)
δ calc CH_2 3.65 (obs 2.4)
Σ Δδ: 1.55

2

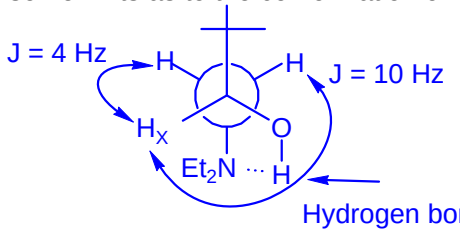
"Nutty compound" (aminal)



δ calc CH 5.2 (obs 3.2)
δ calc CH_2 1.55 (obs 2.4)
Σ Δδ: 2.85

(f) Are there features of the NMR spectrum which provide some hints as to the conformation of **R-07J**?

3 The large difference in the two ^3J couplings suggests a strongly favored conformation - not surprising with a t-butyl group as anchor



Hydrogen bond?
OH chemical shift suggests yes