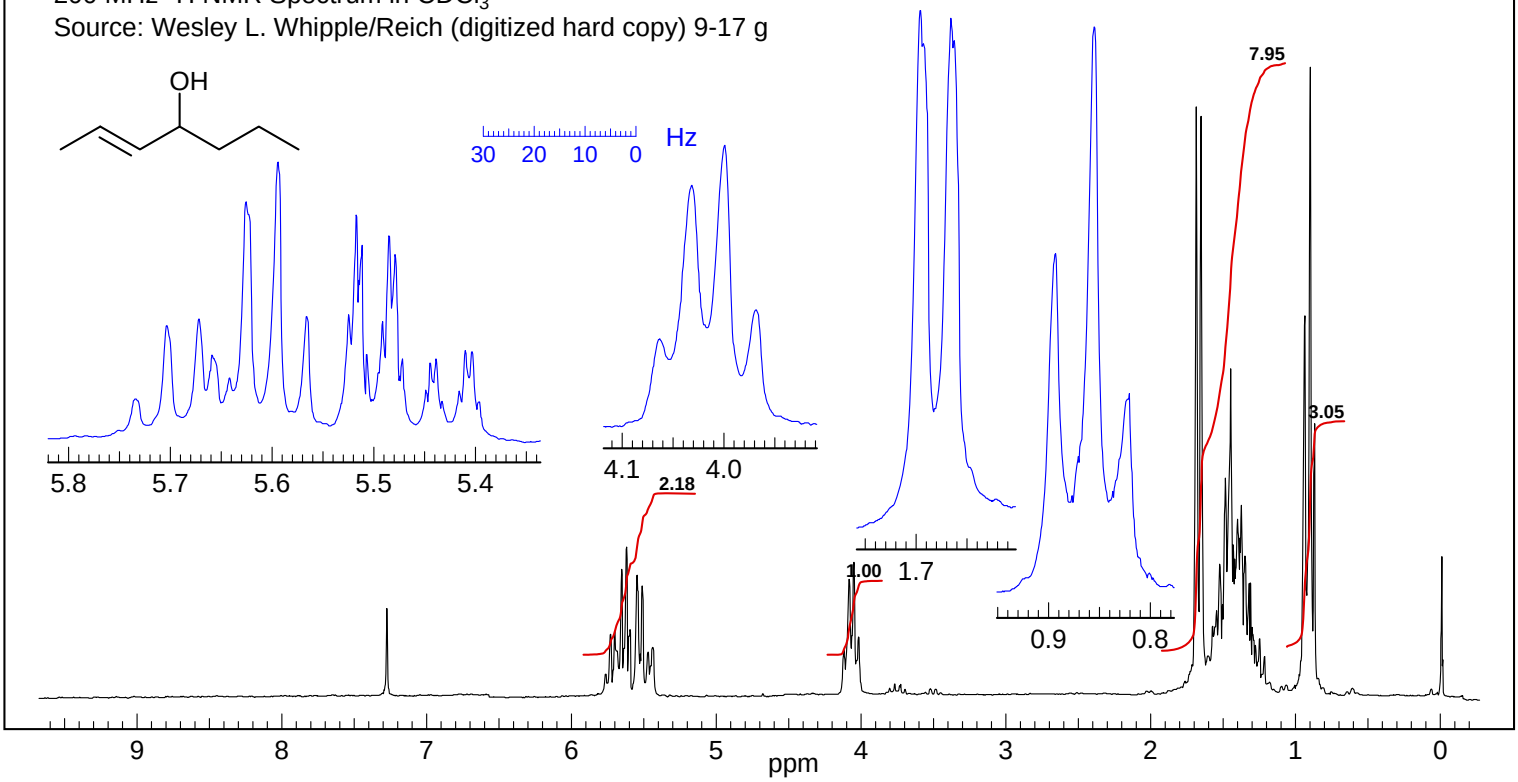
Problem R-00D ($C_7H_{14}O$)

200 MHz ^1H NMR Spectrum in $CDCl_3$

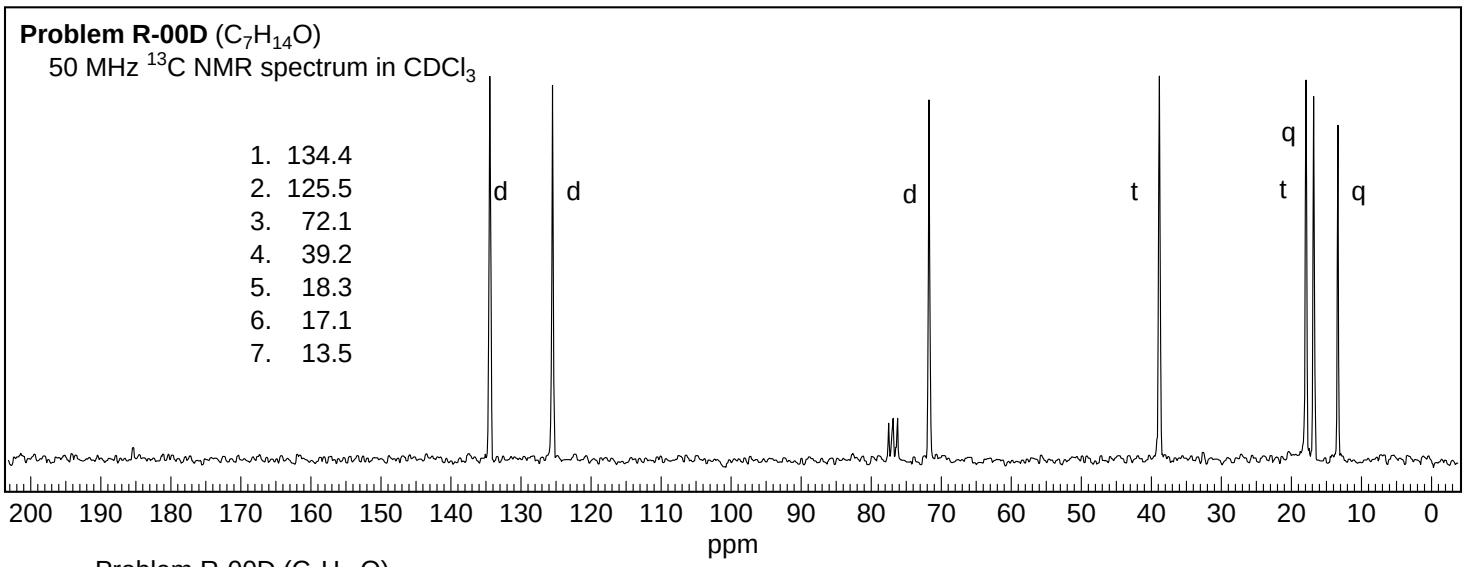
Source: Wesley L. Whipple/Reich (digitized hard copy) 9-17 g



Problem R-00D ($C_7H_{14}O$)

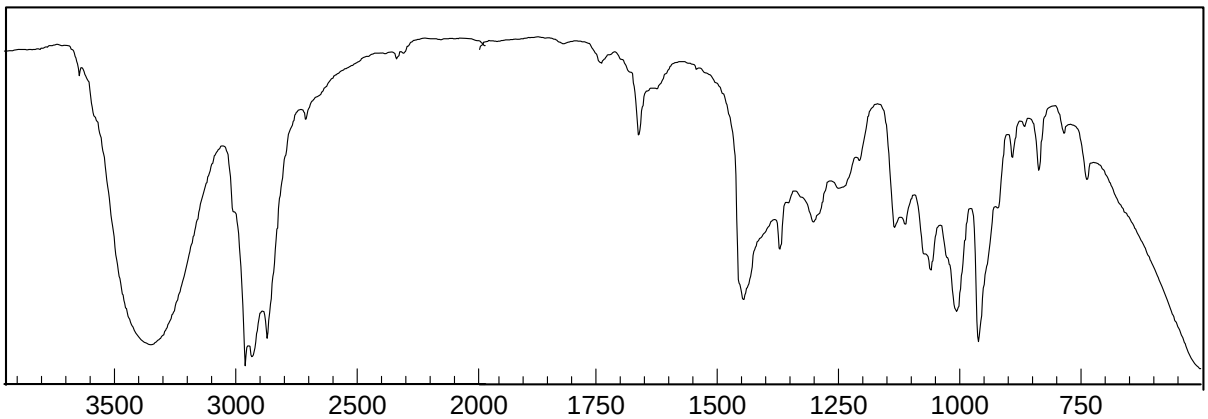
50 MHz ^{13}C NMR spectrum in $CDCl_3$

1. 134.4
2. 125.5
3. 72.1
4. 39.2
5. 18.3
6. 17.1
7. 13.5



Problem R-00D ($C_7H_{14}O$)

Infrared Spectrum neat



PLT ex-1-2000-g.plt

Problem R-00D ($C_7H_{14}O$). Determine the structure of **R-00D** from the ^1H NMR, ^{13}C NMR and IR spectra provided.

(a) DBE____

(b) What information can you obtain from the IR spectrum (give frequency and peak assignment).

(c) Interpret the ^{13}C NMR spectrum, showing any part structures that can be identified. After you have decided on a structure, assign the resonances by writing δ values next to the individual carbons.

(d) Analyze the ^1H NMR spectrum. For each of the signals listed below, report the multiplet structure in the standard format (e.g., 0.0 δ, dtd, J = 0.0, 0.0, 0.0 Hz, 2H) and any part structure you could obtain from the signal(s).

1.0 δ _____

1.5 δ _____

1.7 δ _____

4.0 δ _____

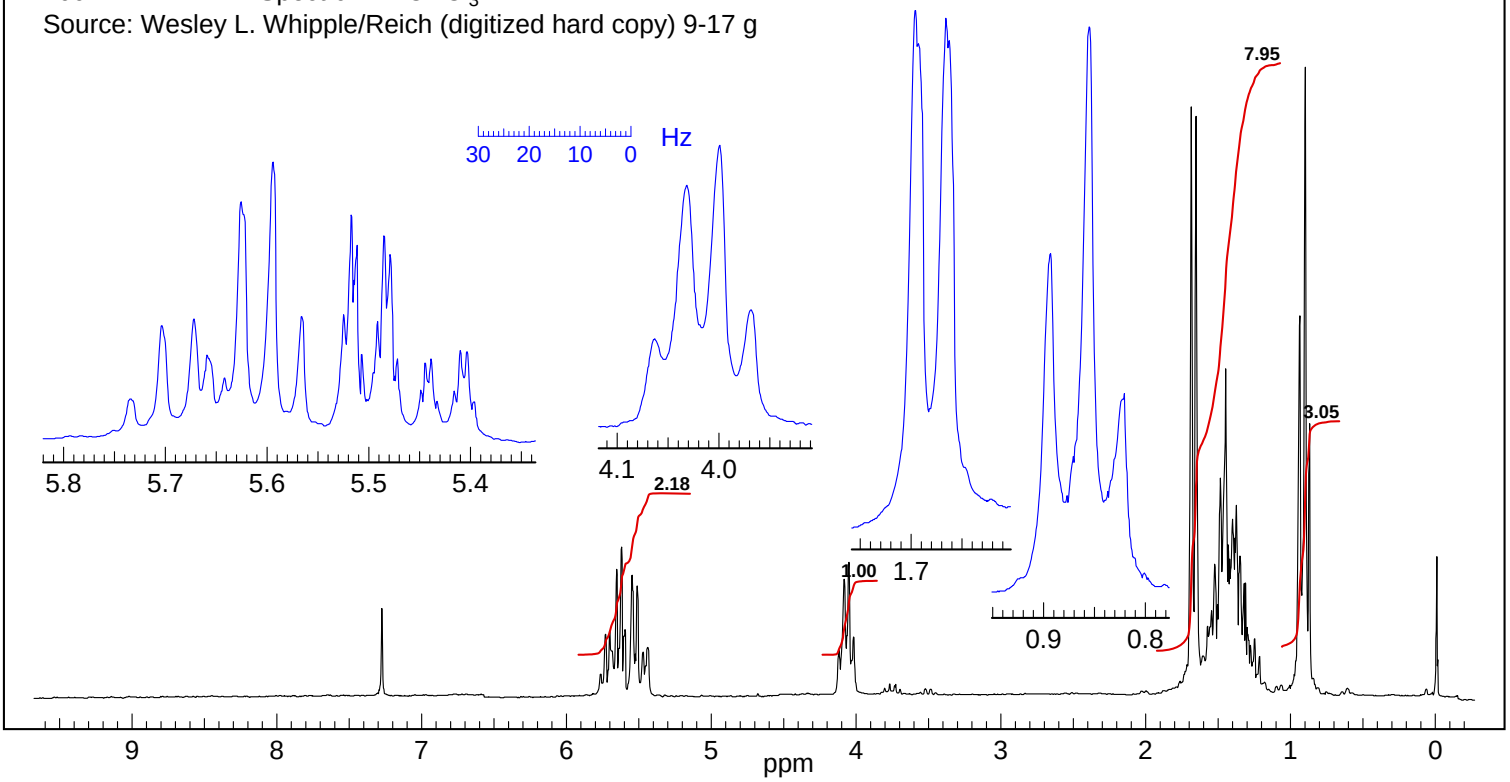
5.5 δ _____

(e) Give your answer below.

Problem R-00D ($C_7H_{14}O$)

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

Source: Wesley L. Whipple/Reich (digitized hard copy) 9-17 g



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50 MHz ^{13}C NMR spectrum in $CDCl_3$

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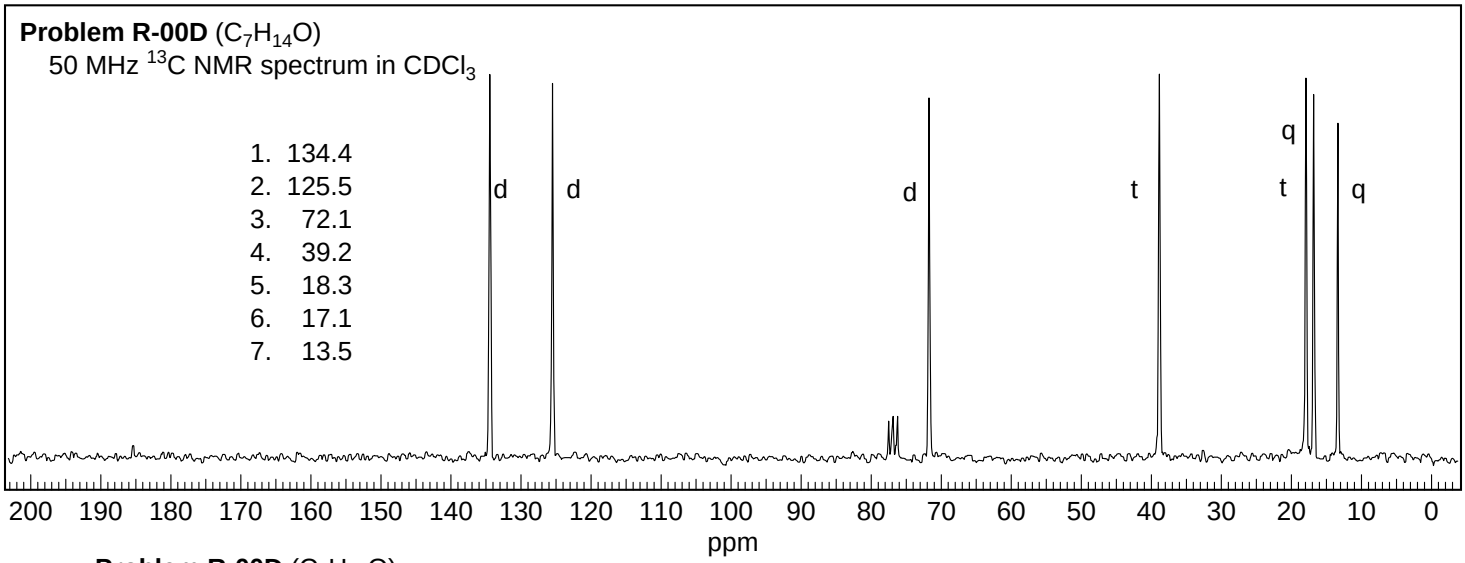
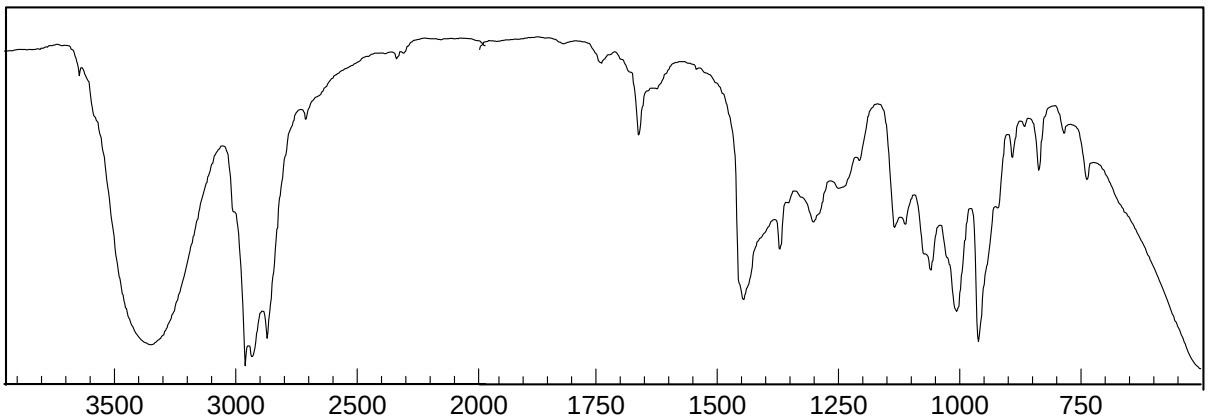


Problem R-00D ($C_7H_{14}O$)

Infrared Spectrum neat



PLT ex-1-2000-g.plt

Problem R-00D ($C_7H_{14}O$). Determine the structure of **R-00D** from the ^1H NMR, ^{13}C NMR and IR spectra provided.

2 (a) DBE 1

(b) What information can you obtain from the IR spectrum (give frequency and peak assignment).

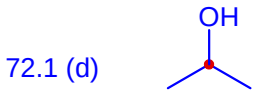
3350 cm^{-1} broad peak means H-bonded OH

1660 cm^{-1} C=C stretch

4 970 cm^{-1} possible *trans* double bond

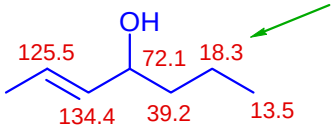
No peak 1700-1800 not a ketone or aldehyde

(c) Interpret the ^{13}C NMR spectrum, showing any part structures that can be identified. After you have decided on a structure, assign the resonances by writing δ values next to the individual carbons.



125 (d) 133 (d) H-C=C-H

6 Rest are aliphatic: CH_3, CH_3, CH_2, CH_2



Calc this chemical shift:

-2.1

9.1 (α)

9.1 (

9.4 (β)

-2.5 (γ_C)

-4.0 (γ_O)

19.0

(d) Analyze the ^1H NMR spectrum. For each of the signals listed below, report the multiplet structure in the standard format (e.g., 0.0 δ, dtd, J = 0.0, 0.0, 0.0 Hz, 2H) and any part structure you could obtain from the signal(s).

1.0 δ — 0.86 δ, t, *J* = 7 Hz, 3H CH_3-CH_2-

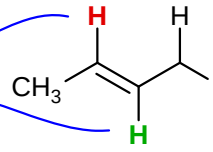
1.5 δ — 1.5 δ, m, 5H

1.7 δ — 1.68 δ, dd, *J* = 7, 1 Hz, 3H CH_3-CH=CH — Chem shift requires allylic CH_3 group

6 4.0 δ — 4.02 δ, q (distorted, maybe dt), *J* = 7Hz, 1H CH_3-C(①OH)-C or CH_2(②OH)-C-CH, H

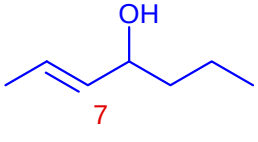
Common error: taking only (1) into account

5.5 δ — 5.63 δ, dq, *J* = 16, 7 Hz, 1H; 5.47 δ, ddq, *J* = 16, 7, 1 Hz



(e) Give your answer below.

7



Other structures proposed: