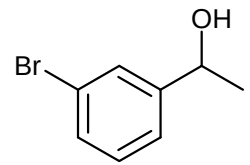
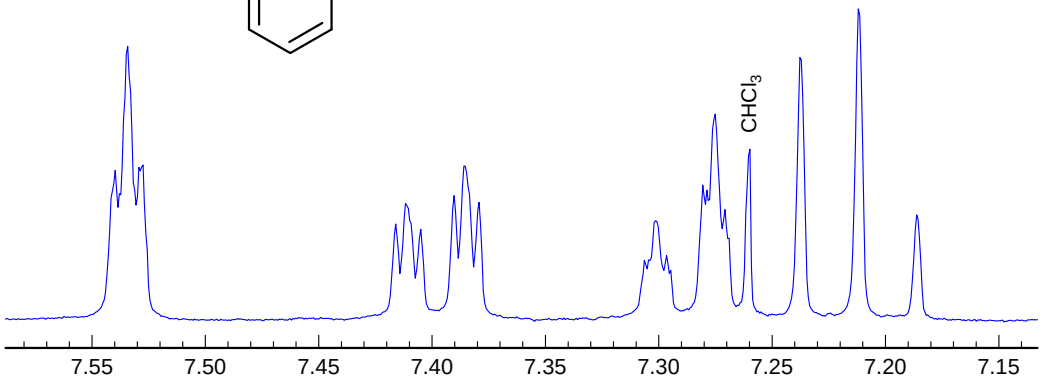
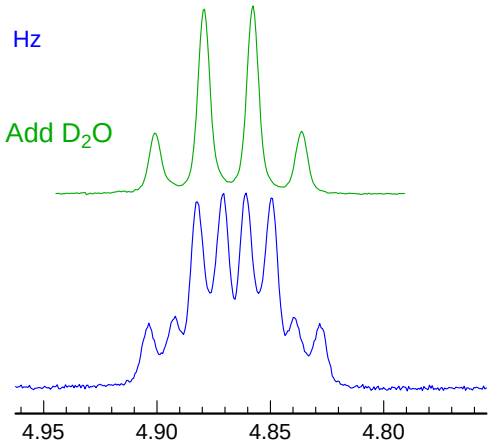
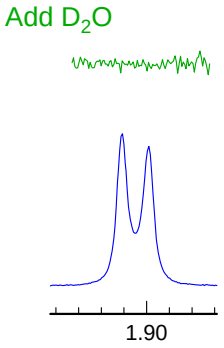
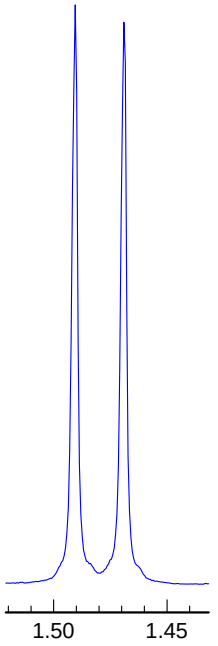
Problem R-00A (C_8H_9BrO).
300 MHz ^1H NMR Spectrum in $CDCl_3$.
Source: Marty Bevan/Reich 10/30 g









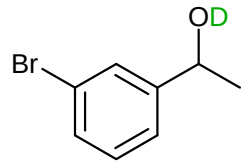


PLT ex-1-2000-g.plt

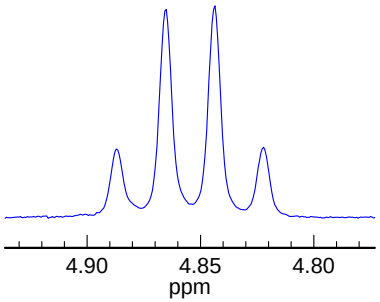
Problem R-00A (C_8H_9BrO).

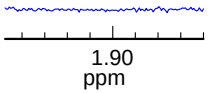
300 MHz ^1H NMR Spectrum in $CDCl_3$ with D_2O.

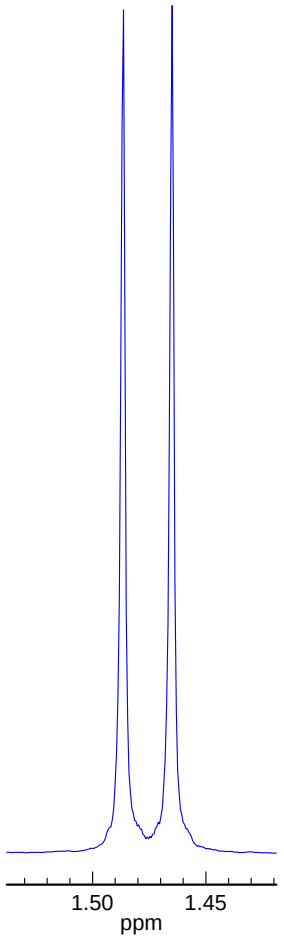
Source: Marty Bevan/Reich 10/30



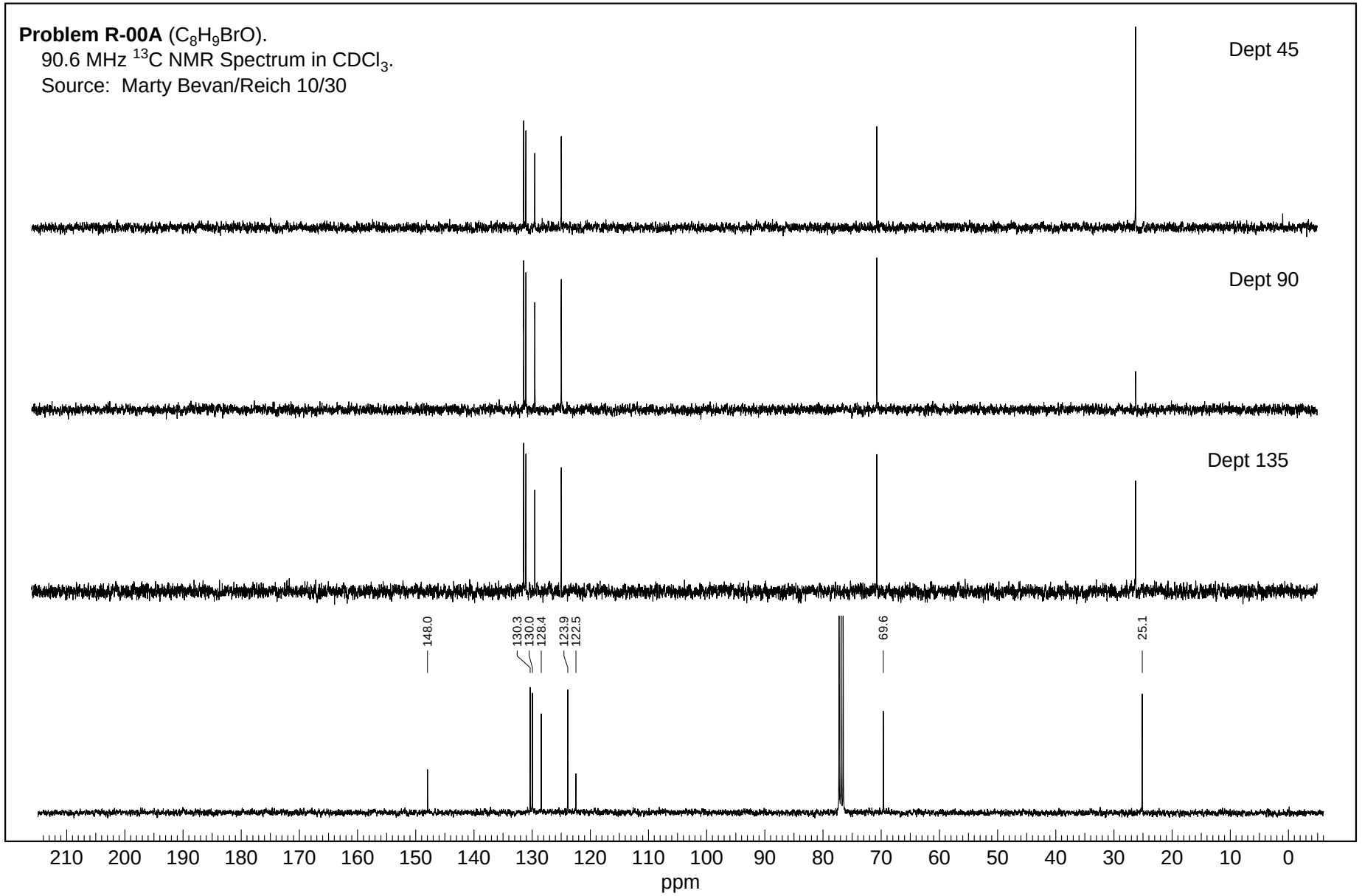
Add D_2O







PLT ex-1-2000-g.plt



PLT ex-1-2000-g.plt

Problem R-00A (C_8H_9BrO). You are provided the ^1H NMR spectrum of a compound, and asked to interpret the NMR spectrum, and determine the structure or structures. Show the chemical shift and multiplet structure in the form: 0.0 δ, dtd, J = 0.0, 0.0, 0.0 Hz, 1H . You may use first order analysis.

(a) DBE _____

(b) Analyze the multiplets δ 1-5. Two of the multiplets are shown after a drop of D_2O was added to the sample (with shaking of the sample). Interpret this behavior, and provide part structure(s).

A δ 1.5 _____

B δ 1.9 _____

C δ 4.9 _____

(c) Interpret the signals between δ 7.15 and δ 7.55.

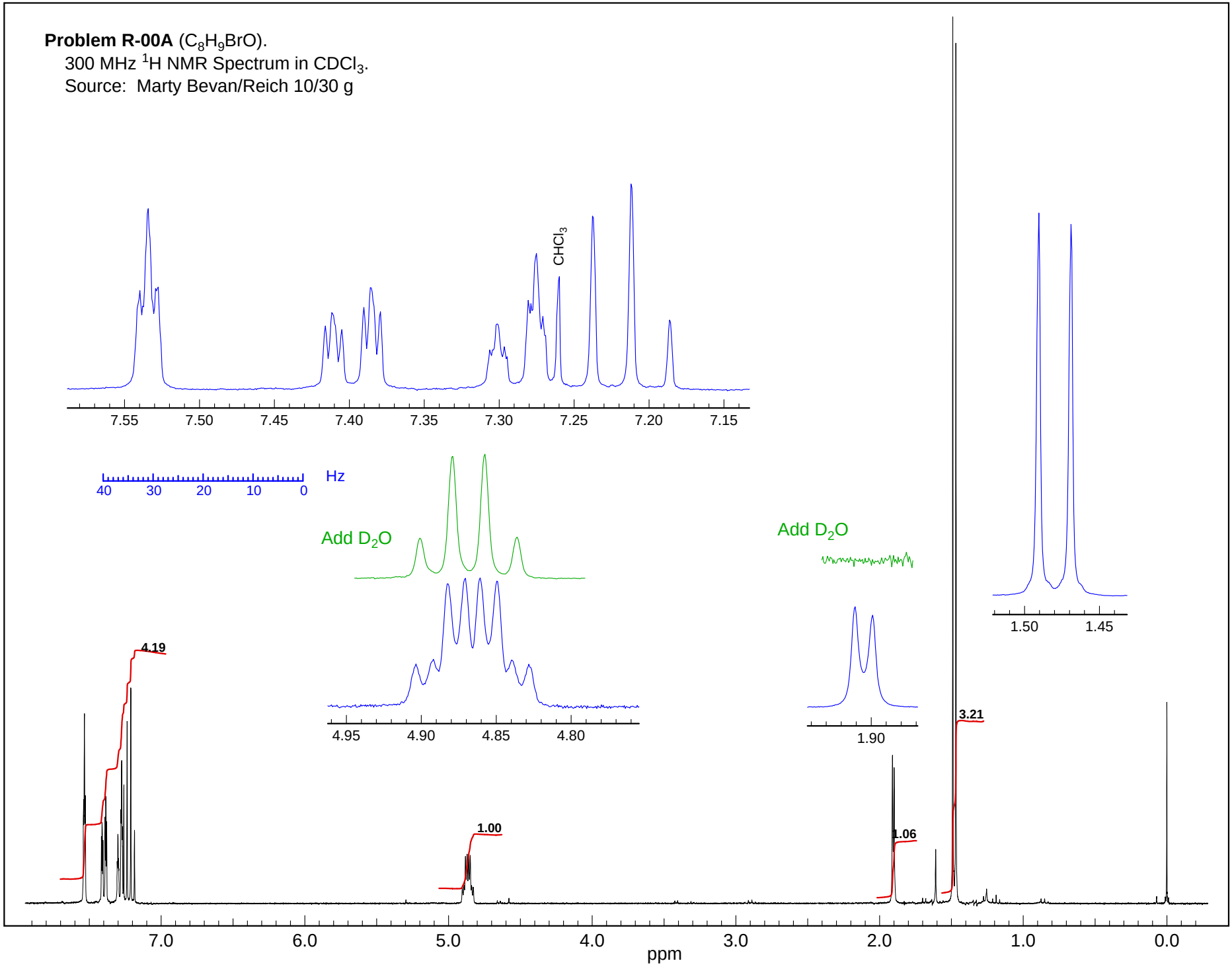
D_____

E_____

F_____

G_____

(d) Draw the structure of **R-00A** below. If more than one structure fits the data, draw them, but circle your best choice. Assign the protons (label them with the letters A-G. If any assignments are ambiguous, indicate the basis for your choice.



PLT ex-1-2000-g.plt

Problem R-00A (C_8H_9BrO). You are provided the ^1H NMR spectrum of a compound, and asked to interpret the NMR spectrum, and determine the structure or structures. Show the chemical shift and multiplet structure in the form: 0.0 δ, dtd, J = 0.0, 0.0, 0.0 Hz, 1H . You may use first order analysis.

2 (a) DBE 4

(b) Analyze the multiplets δ 1-5. Two of the multiplets are shown after a drop of D_2O was added to the sample (with shaking of the sample). Interpret this behavior, and provide part structure(s).

A δ 1.5 δ 1.48, d, *J* = 7 Hz, 3H CH_3-C(H)-

5 B δ 1.9 δ 1.91, d *J* = 3.5 Hz, 1H must be CH_3-C(OH)(H)- since D_2O causes it to disappear

C δ 4.9 δ 4.86, qd *J* = 6.5, 4 Hz, 1H must be CH_3-C(OH(D))(H)- since D_2O causes splitting to disappear

(c) Interpret the signals between δ 7.15 and δ 7.55.

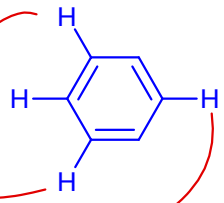
These are the aromatic protons in a 1,2,3,5-relationship

D δ 7.21, t (leaning towards 7.28 multiplet), *J* = 7.8 Hz, 1H

E δ 7.28, dt (dtd?), *J* = 8, 3, (1?} Hz, 1H

5 F δ 7.40, ddd, *J* = 7.8, 2, 1.5 Hz, 1H

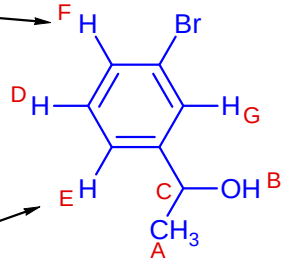
G δ 7.53, t (td?), *J* = 3.5, (1?) Hz, 1H



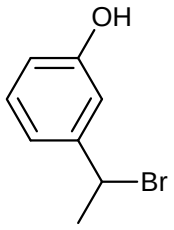
(d) Draw the structure of **R-00A** below. If more than one structure fits the data, draw them, but circle your best choice. Assign the protons (label them with the letters A-G. If any assignments are ambiguous, indicate the basis for your choice.

Calc.
Base: 7.36
p-CH_2OH:-0.07
o-Br: 0.13
7.42
8 Obs: 7.40

Calc.
Base: 7.36
o-CH_2OH: -0.07
p-Br: -0.08
7.22
Obs: 7.28



8



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