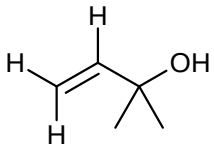
Problem R-09N ($C_5H_{10}O$)

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

Source: Aldrich Spectra Collection/Reich g

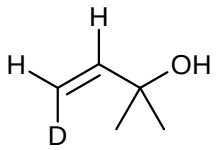


PLT ex-3-2009-10-gq.plt

Problem R-09N C_5H_9DO

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

Source: Ken Yelm/Reich (digitized hard copy)



PLT ex-3-2009-10-gq.plt

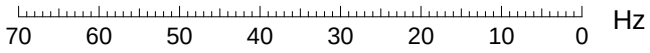
Problem R-09N (C_5H_9DO) Yes, that's a deuterium. Determine the structure from the 200 MHz ^1H NMR spectrum.

(a) DBE_____ (b) Interpret the multiplets at δ 4.95 and δ 5.95. Report coupling in the standard format ($^nJ_{x-y}$ = 00 Hz). Show part structure(s) suggested by these peaks

δ 4.95

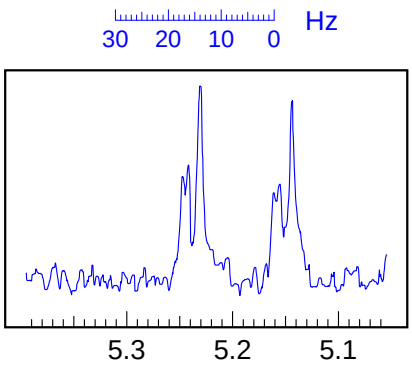
δ 5.95

(c) On the Hz scale below sketch what the proton at δ 5.95 would look like in the undeuterated compound ($C_5H_{10}O$)



(d) Draw the structure of R-09N. If more than one structure is possible, then draw them, but circle the one you prefer.

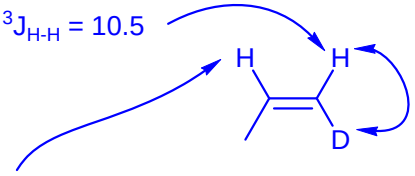
(e) The boxed inset between δ 5.1 and 5.3 (reproduced below) is an 8x vertical expansion. Suggest what these small impurities might be due to, and assign the peaks..



Problem R-09N (C_5H_9DO) Yes, that's a deuterium. Determine the structure from the 200 MHz ^1H NMR spectrum.

1 (a) DBE **1** (b) Interpret the multiplets at δ 4.95 and δ 5.95. Report coupling in the standard format ($^nJ_{x\text{-}y}$ = 00 Hz). Show part structure(s) suggested by these peaks

δ 4.95 d $^3J_{H\text{-}H}$ = 10.5



The protons must be cis on the double bond to give a 10 Hz coupling

$^2J_{HD}$ is too small to detect (ca 0.4 Hz)

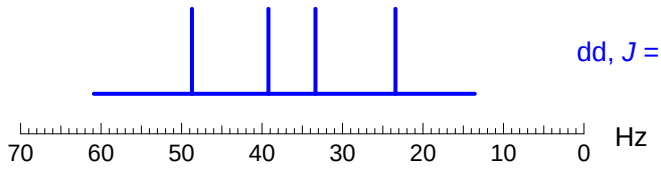
5 δ 5.95 d 1:1:1 t, $^3J_{H\text{-}H}$ = 10.5, $^3J_{H\text{-}D}$ = 2.5 Hz

The 1:1:1 triplet 2.5 Hz is J_{HD}, J_{HH} = 2.5 x 100/15.35 = 16.3 Hz

$J_{HH} = J_{HD} \times \gamma_H/\gamma_D$

(c) On the Hz scale below sketch what the proton at δ 5.95 would look like in the undeuterated compound ($C_5H_{10}O$)

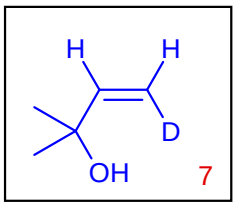
3

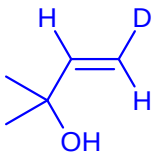


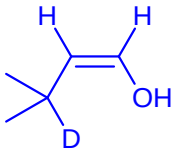
dd, J = 16, 10 Hz

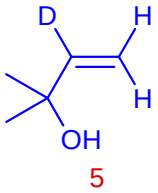
(d) Draw the structure of R-09N. If more than one structure is possible, then draw them, but circle the one you prefer.

7

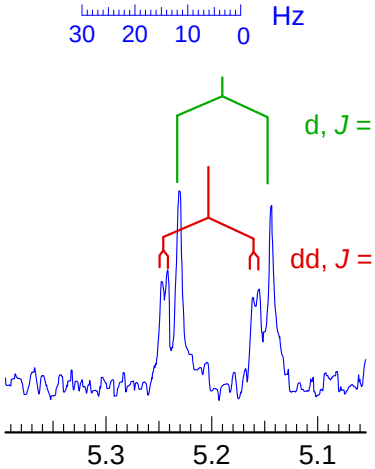




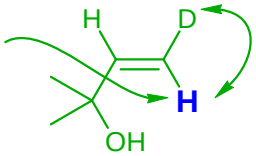




(e) The boxed inset between δ 5.1 and 5.3 (reproduced below) is an 8x vertical expansion. Suggest what these small impurities might be due to, and assign the peaks..



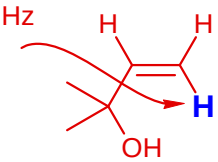
d, J = 16.5 Hz



The impurities are a mixture of the undeuterated compund, and the compound with D in the trans position, about 4% of the sample

$^2J_{H\text{-}D}$ is too small to detect (ca 0.4 Hz)

4 dd, J = 16.5, 1.5 Hz



This is a bit of the undeuterated compound

There is a small H/D isotope shift, with the deuterated compound being slightly upfield of the protio (Δδ 15 ppb)

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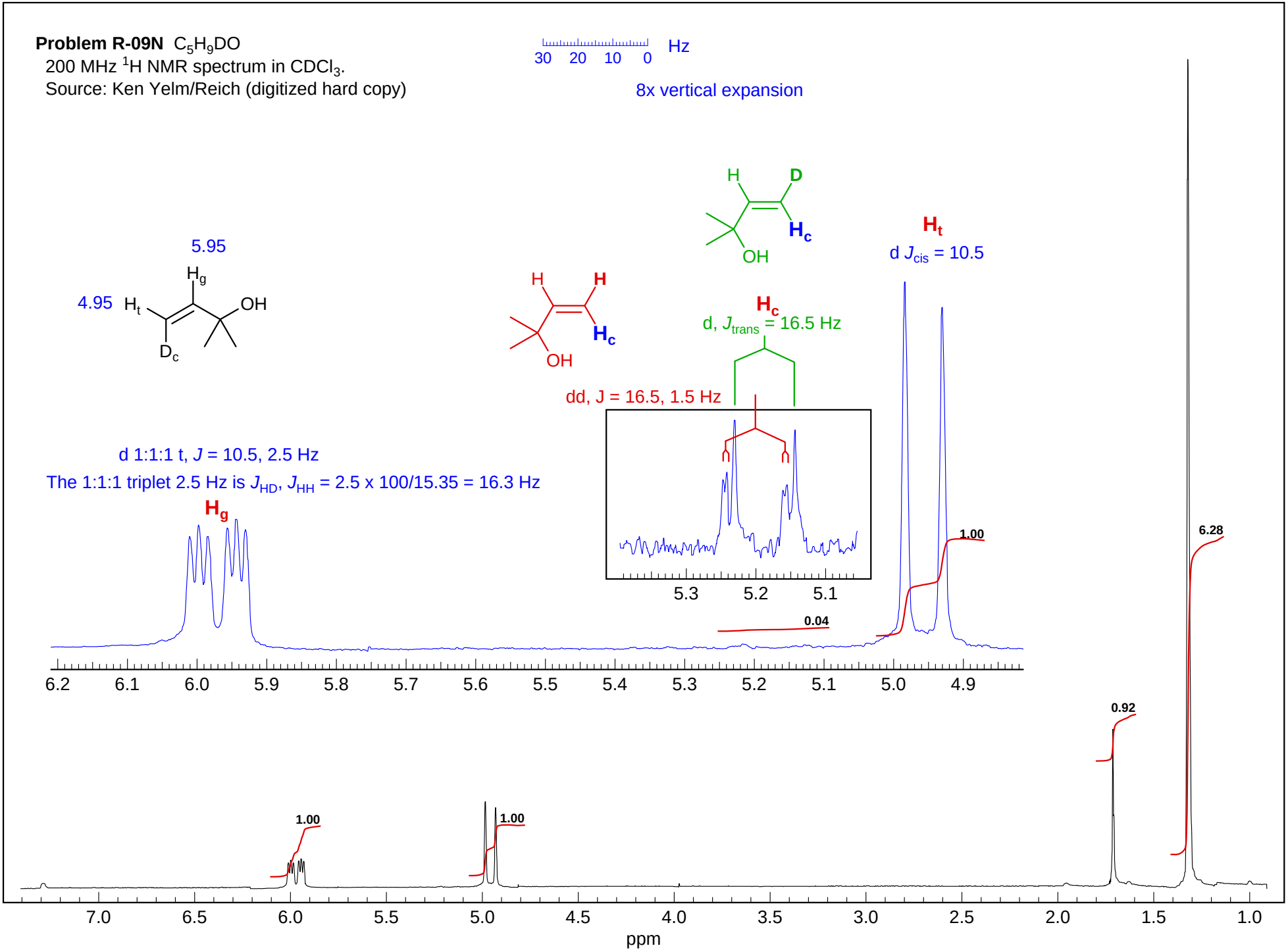

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