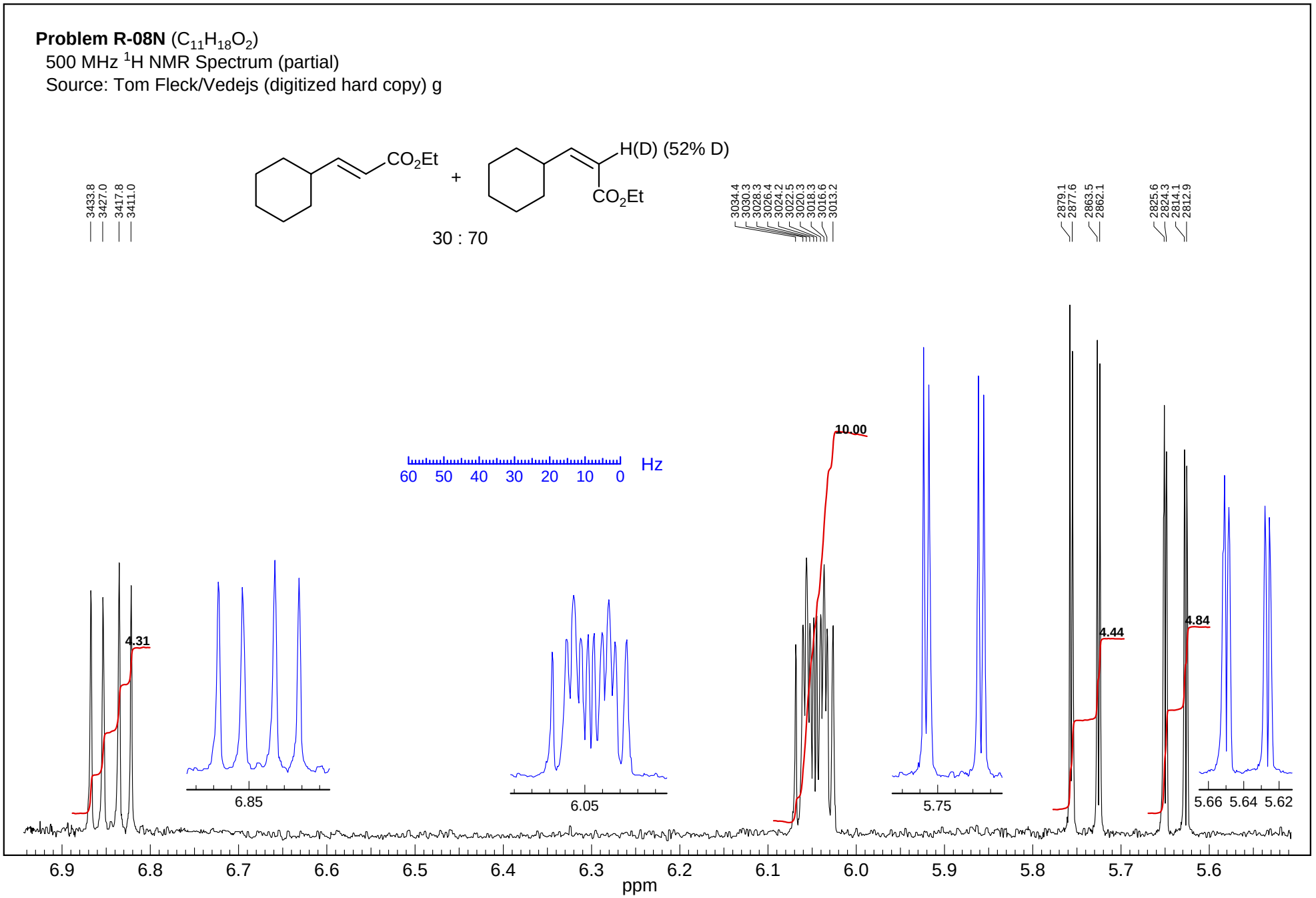
Problem R-08N ($C_{11}H_{18}O_2$)

500 MHz ^{1}H NMR Spectrum (partial)

Source: Tom Fleck/Vedejs (digitized hard copy) g



PLT ex-3-08-09.plt

Problem R-08N ($C_{11}H_{18}O_2$). You are given the partial 500 MHz ^{1}H NMR spectrum of a cis/trans mixture of partially deuterated cyclohexyl acrylates and asked to assign the signals and determine the position of deuteration. **Only one vinyl position of one isomer is partially deuterated**.

(a) Analyze and assign each of the signals listed below. Report multiplicities and couplings in the standard format (there may be more than one signal at a chemical shift position). For each indicate whether it belongs to the cis or the trans isomer.

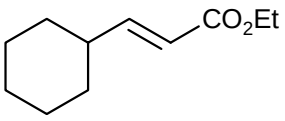
δ 5.64 (cis or trans) _____

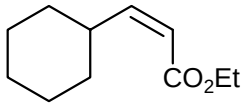
δ 5.74 (cis or trans) _____

δ 6.05 (cis or trans) _____

δ 6.85 (cis or trans) _____

(b) Determine the position and extent of deuteration, as well as the ratio of cis and trans isomers, and indicate this on the structures below. Briefly summarize the evidence.





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500 MHz ^{1}H NMR Spectrum (partial)

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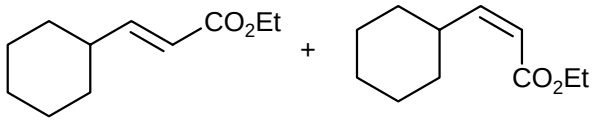


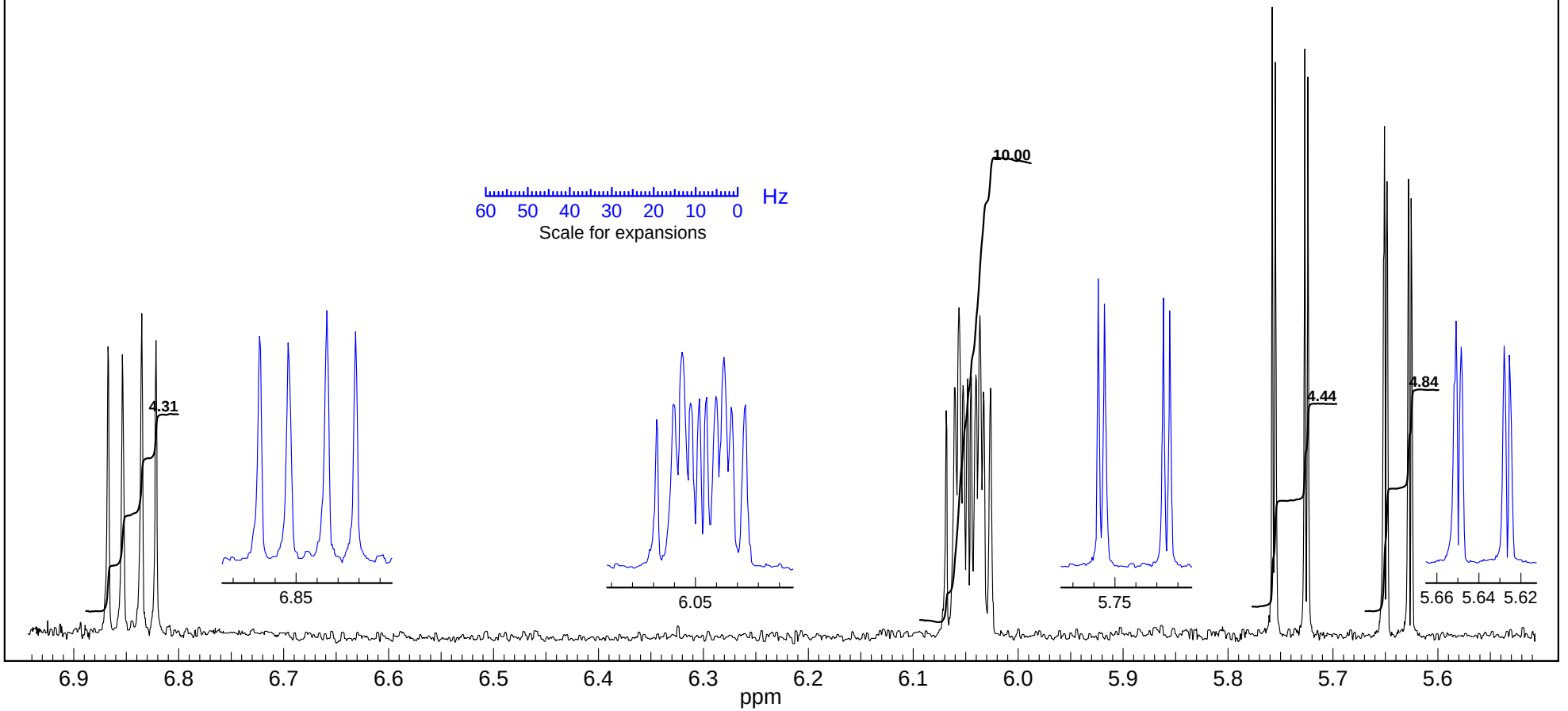
3433.8 3427.0 3417.8 3411.0

3034.4 3030.3 3028.3 3026.4 3024.2 3022.5 3020.3 3018.3 3016.6 3013.2

2879.1 2877.6 2863.5 2862.1

2825.6 2824.3 2814.1 2812.9

One of the four vinyl position is partially deuterated.



PLT ex-3-08-09.plt

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Problem R-08N ($C_{11}H_{18}O_2$). You are given the partial 500 MHz ^{1}H NMR spectrum of a cis/trans mixture of partially deuterated cyclohexyl acrylates and asked to assign the signals and determine the position of deuteration. **Only one vinyl position of one isomer is partially deuterated**.

(a) Analyze and assign each of the signals listed below. Report multiplicities and couplings in the standard format (there may be more than one signal at a chemical shift position). For each indicate whether it belongs to the cis or the trans isomer.

2 δ 5.64 (cis or trans) dd, J = 11, 2 Hz — Cis

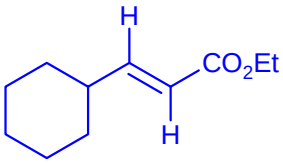
2 δ 5.74 (cis or trans) dd, J = 16, 2 Hz — Trans

5 δ 6.05 (cis or trans) dd, J = 10, 11 Hz + d of 1:1:1 triplets, J = 10, 2.0 Hz — Cis + cis-D

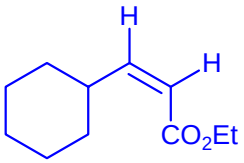
2 δ 6.85 (cis or trans) dd, J = 16, 7 Hz — Trans

(b) Determine the position and extent of deuteration, as well as the ratio of cis and trans isomers, and indicate this on the structures below. Briefly summarize the evidence.

9



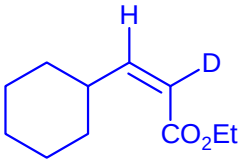
(4.31 + 4.44)/2 = 4.37



4.84

2

3



10.0 - 4.84 = 5.16

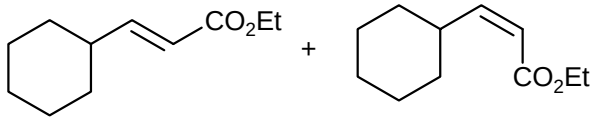
51.6% d

2 30.4% trans

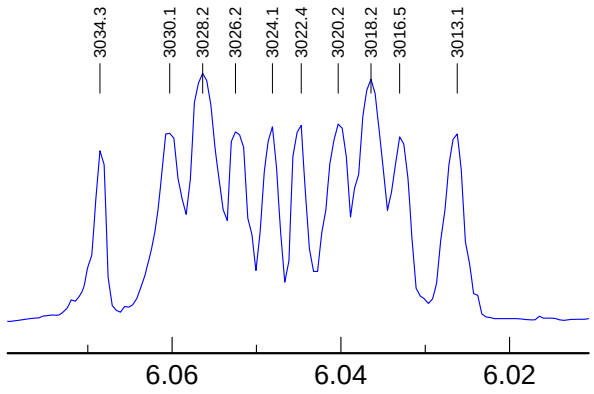
69.6% cis

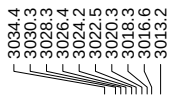
2 Explanation

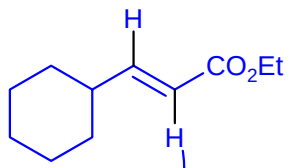
Problem R-08N ($C_{11}H_{18}O_2$)
500 MHz ^{1}H NMR Spectrum (partial)
Source: Tom Fleck/Vedejs

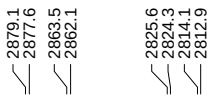


One of the four vinyl position is partially deuterated.

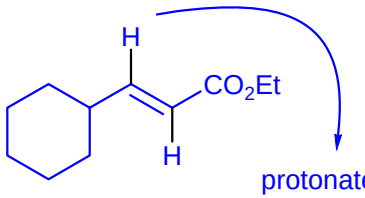




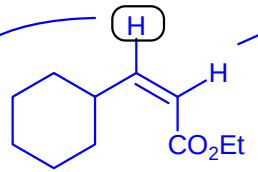




Scale for expansions

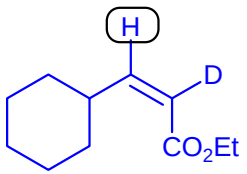


protonated
trans
dd, J = 16, 7 Hz



protonated cis
dd, J = 10, 11 Hz

deuterated cis



protonated
trans
dd, J = 16, 2 Hz

protonated
cis
dd, J = 11, 2 Hz

d (10 Hz) of 1:1:1 triplets (2 Hz)

PLT ex-3-08-09.plt