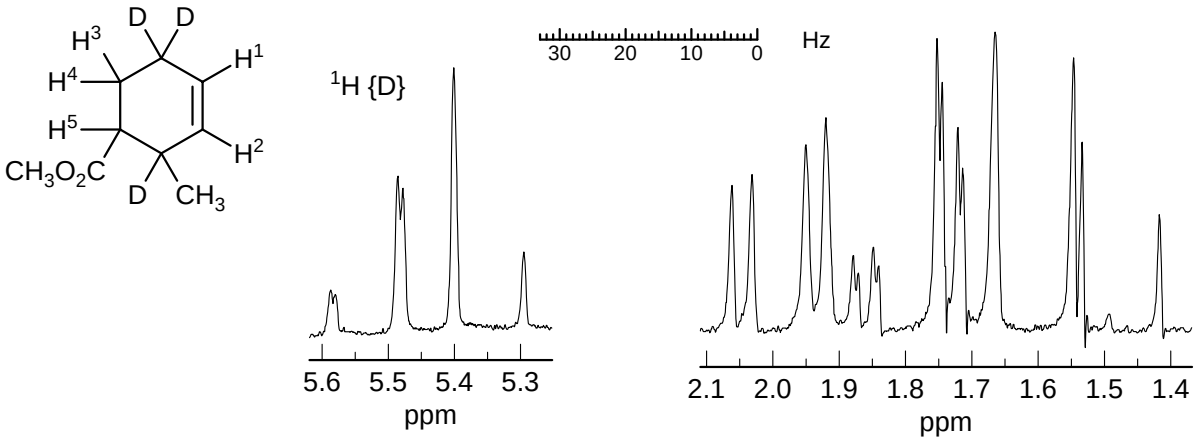
Problem R-84l ($C_9H_{14}O_2$). Shown below is the partial NMR spectrum (100 MHz, CS_2 solvent, deuterium decoupled) of a deuterated cyclohexene derivative (the CH_3 resonances are not shown). Source: *Org. Magn. Res.* **1973**, *5*, #10, Spect #0635 (digitized hard copy) g



(a) Provide a complete interpretation of the signals shown. Give chemical, shifts and coupling constants. Assume first order analysis.

H^1 _____ δ, J = _____ Hz, coupled to: _____

H^2 _____ δ, J = _____ Hz, coupled to: _____

H^3 _____ δ, J = _____ Hz, coupled to: _____

H^4 _____ δ, J = _____ Hz, coupled to: _____

H^5 _____ δ, J = _____ Hz, coupled to: _____

(b) Using this information, draw a good representation of the conformation of compound **R-84l**. Label the hydrogens (1, 2, etc.) of your structure. Are the CH_3 and CO_2CH_3 groups cis or trans? (Hint: which group is larger in a cyclohexane?)

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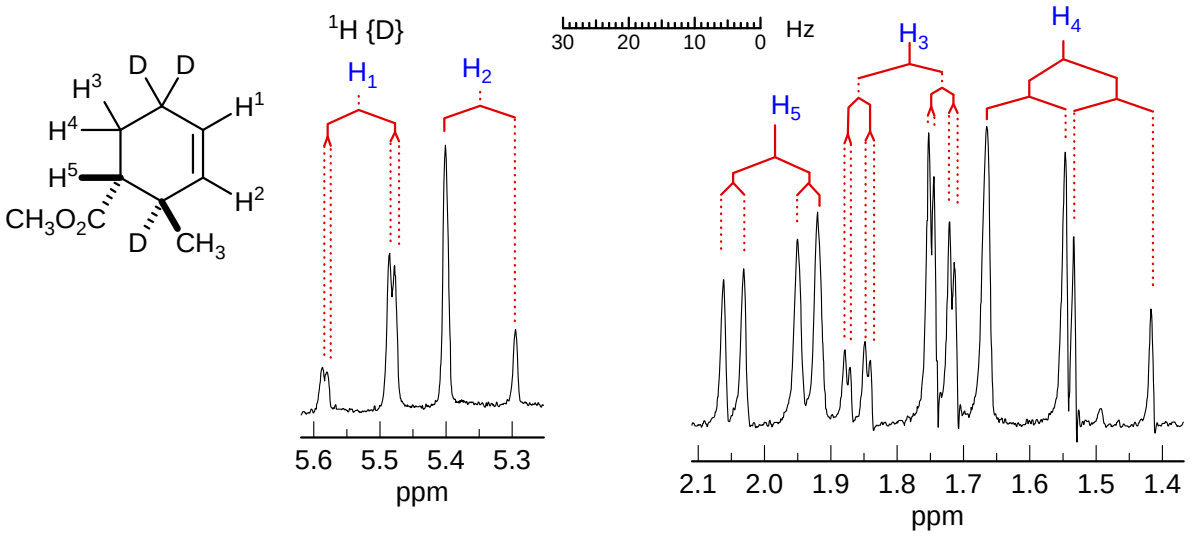


(a) Provide a complete interpretation of the signals shown. Give chemical, shifts and coupling constants. Assume first order analysis.

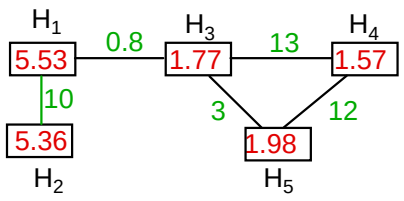
H^1	5.53	δ, J =	10, 0.8	Hz, coupled to:	H_2, H_3
H^2	5.36	δ, J =	10	Hz, coupled to:	H_1
H^3	1.77	δ, J =	13, 3, 0.8	Hz, coupled to:	H_4, H_5, H_2
H^4	1.57	δ, J =	13, 12	Hz, coupled to:	H_3, H_5
H^5	1.98	δ, J =	12, 3	Hz, coupled to:	H_4, H_3

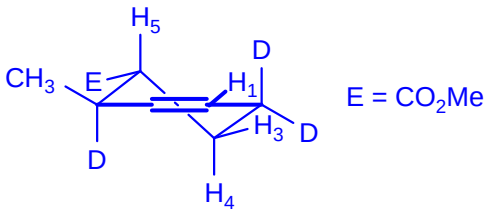
(b) Using this information, draw a good representation of the conformation of compound **R-84l**. Label the hydrogens (1, 2, etc.) of your structure. Are the CH_3 and CO_2CH_3 groups cis or trans? (Hint: which group is larger in a cyclohexane?)

Coupling scheme:

A_{Me} = 1.70

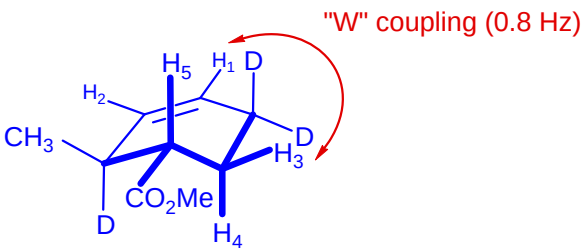
A_{COOMe} = 1.27





E = CO_2Me

We only know that H_5 must be axial, because of the large coupling to H_4, thus the CO_2Me group is equatorial. Since Me is larger than CO_2Me in a cyclohexane, we assume that this is also the case for cyclohexene, thus placing the methyl equatorial. If the methyl were axial, the ring would flip, H_5 would be equatorial, and the NMR spectrum would not fit the structure. Thus the two substituents are *trans*.



Problem R-84I

Treating this spectrum as first order (AMX analysis) leads to small errors in J_{35} (AMX: 3.0, actual 2.1 Hz) and J_{45} (AMX: 12.0, actual: 12.6 Hz). As is always the case, the first order couplings are in error in the direction of average of the two couplings involved.