

Vicinal Deuterium Perturbations on Hydrogen NMR Chemical Shifts in Cyclohexanes

Daniel J. O'Leary,[†] Damian G. Allis,[‡] Bruce S. Hudson,[‡] Shelly James,[‡]
Katherine B. Morgera,[‡] and John E. Baldwin^{*‡}

*Department of Chemistry, Pomona College, Claremont, California 9171-6338, and the
Department of Chemistry, Syracuse University, Syracuse, New York 13244-4100*

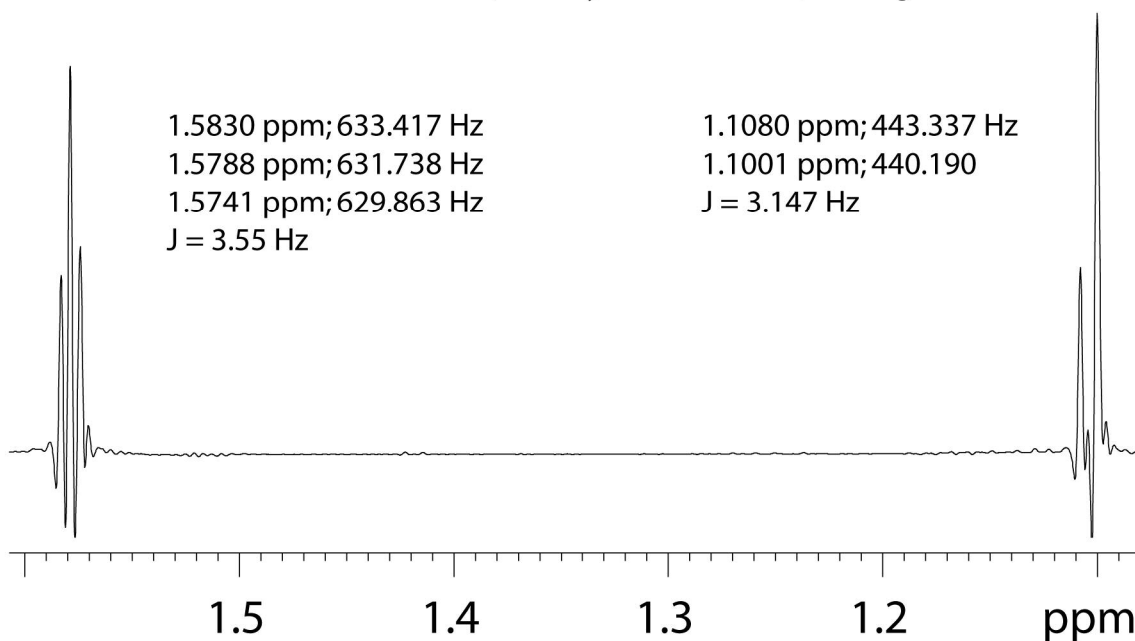
E-mail: jbaldwin@syr.edu

[†]Pomona College [‡]Syracuse University

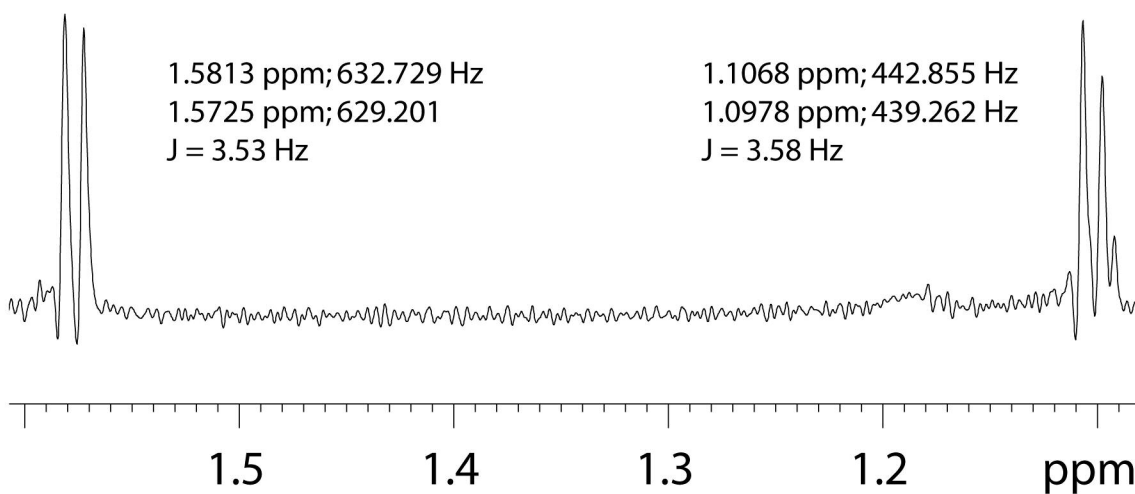
Supporting Information: Two pages of low-temperature $^1\text{H}\{^2\text{H}\}$ NMR spectra at 400.13 MHz for the cis and trans isomers of 1,2,3,3,4,4,5,5,6,6- d_{10} -cyclohexane and d_{11} -cyclohexane, and full citation for reference 28.

Spectra recorded 8/10/07. The three values recorded for the ax H and eq H vicinal coupling constant for the cis isomer are 3.55, 3.53, and 3.58 Hz (3.55 ± 0.025 Hz). The axial H resonance for the trans isomer is $(3.55 - 3.15) = 0.4$ Hz downfield from the calculated upfield component of the axial H in the cis isomer.

mixture of cis- and trans-1,2-H₂-cyclohexane-d₁₀, -86 deg C in CS₂

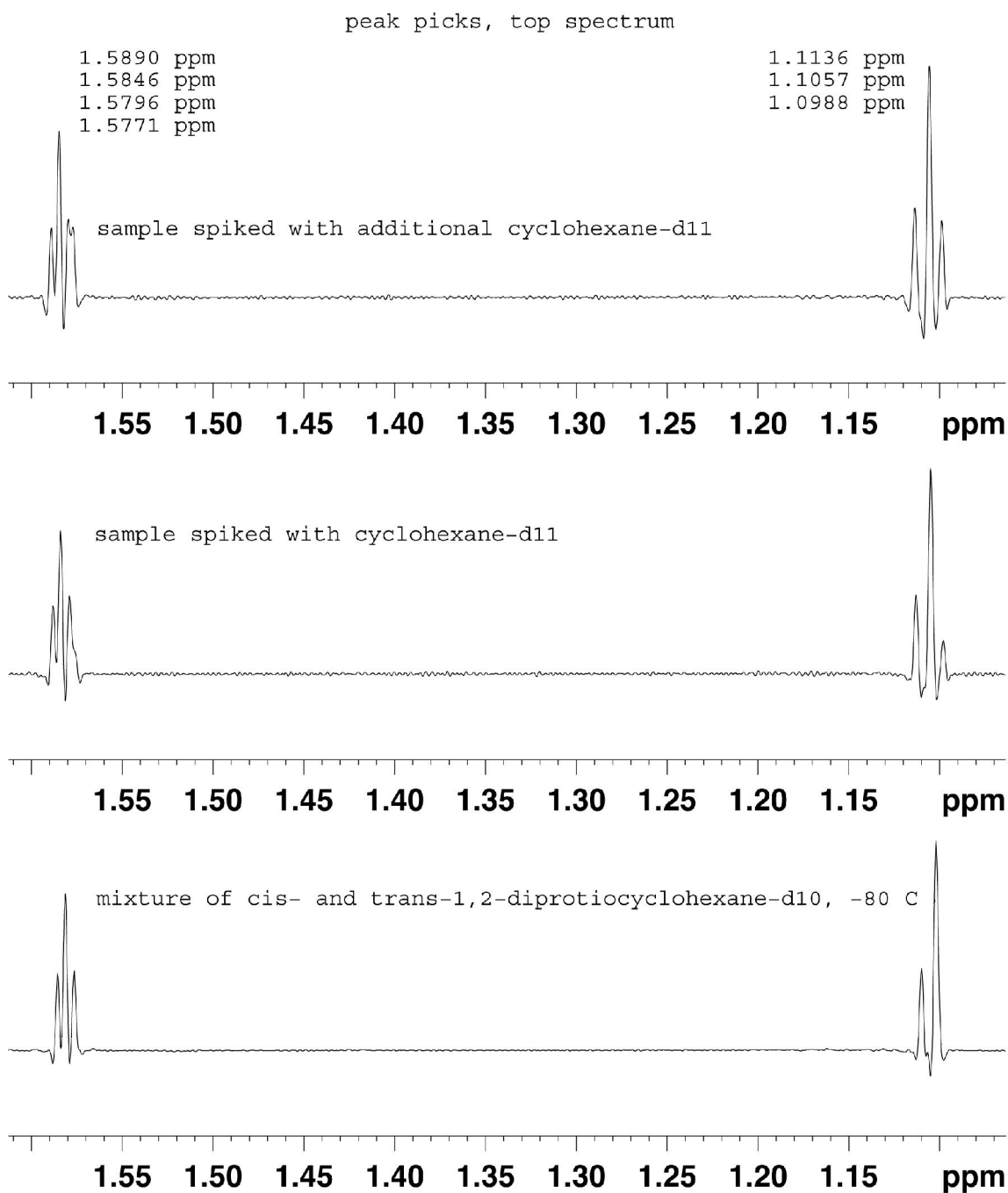


pure cis-1,2-H₂-cyclohexane-d₁₀, -86 deg C in CS₂



Spectra recorded 11/14/07. A 1:1 mixture of the cis and trans isomers of 1,2,3,3,4,4,5,5,6,6- d_{10} -cyclohexane (bottom of graphic); that mixture plus a spike of d_{11} -cyclohexane (middle spectrum); the labeled cyclohexanes after the addition of more d_{11} -cyclohexane (top spectrum). Compare Figure 1.

cyclohexane- d_{11} spike expts
dan o'leary, pomona college
11-14-07



Full citation for reference 28:

Gaussian 03, Revision B.03: Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. Gaussian, Inc., Pittsburgh PA, 2003.