

Hyperconjugation in Trialkylboranes Shown by Indirect Nuclear Spin-Spin Coupling Constants. Experimental Data and Density Functional Theory (DFT) Calculations

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Trimethylborane (**1**), triethylborane (**2**), 1,3-dimethyl-1-boracyclopentane (**3**), 1-methyl-1-boracyclohexane (**4**), 9-methyl- and 9-ethyl-9-borabicyclo[3.1.1]nonane [**5(Me)** and **5(Et)**], and 1-boraadamantane (**6**) were studied by ¹¹B and ¹³C NMR spectroscopy with respect to coupling constants ¹*J*(¹³C, ¹¹B) and ¹*J*(¹³C, ¹³C). Results of DFT calculations at the B3LYP/6-311+g(d,p) level of theory show satisfactory agreement with the experimental data. Hyperconjugation arising from C-C σ bonds adjacent to the tricoordinate boron atom is indicated, in particular for 1-boraadamantane (**6**), by the optimised calculated structures, and by the experimental and calculated data ¹*J*(¹³C, ¹³C). The calculated magnitude of ¹*J*(¹³C, ¹H) for carbon atoms adjacent to boron becomes significantly smaller if the optimised structures suggest hyperconjugative effects arising from these C-H bonds.

Key words: Trialkylboranes, Coupling Constants, ¹³C NMR, DFT, ¹¹B NMR Calculations