Indirect nuclear spin-spin coupling constants $^nJ(1^{11}B, ^1H)$ and $^nJ(1^{11}B, 1^{11}B)$ in Some Boron Hydrides - Density Functional Theory (DFT) Calculations

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Dedicated to Professor Hubert Schmidbaur on the occasion of his 70th birthday

Indirect nuclear spin-spin coupling constants $J(1^{11}B, ^1H)$ and $J(1^{11}B, 1^{11}B)$ in neutral and anionic boron hydrides 1 – 17, calculated at the B3LYP/6-311+G(d,p) level of theory, are in good agreement with experimental data if available. This is shown for $[BH_4]^{-}$ (1), $B_2H_6$ (2), $B_3H_{10}$ (3), $B_5H_9$ (4), or $[B_2H_7]^{-}$ (12). The calculations can be used to obtain values for those coupling constants for which experimental information is hardly accessible. This applies to complex spin systems involving the quadrupolar $^{11}B$ nuclei such as in $[B_6H_6]^{2-}$ (11), to fast dynamic processes such as in $B_6H_{10}$ (5), $[B_5H_8]^{-}$ (10), $[B_6H_7]^{-}$ (11-H), $[B_3H_8]^{-}$ (13), $Be(BH_3)_2$ (14), ($\eta^5-C_5H_5)BeBH_4$ (15), $Be(B_3H_8)_2$ (16), $Me_2AlB_3H_8$ (17), or to instable species such as $[B_2H_6]^{2-}$ (6), $B_2H_4$ (7), $B_3H_7$ (8), and $B_4H_8$ (9). The experimental $^{11}B$ NMR spectrum reported in the literature for the dianion 6 does not resemble the spectrum predicted on the basis of the calculated coupling constants.

Key words: Boranes, Hydroborate Anions, NMR, Coupling Signs, DFT Calculations