

Indirect Nuclear Spin-Spin Coupling Constants ${}^nJ({}^{11}\text{B}, {}^1\text{H})$ and ${}^nJ({}^{11}\text{B}, {}^{11}\text{B})$ 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 $J({}^{11}\text{B}, {}^1\text{H})$ and $J({}^{11}\text{B}, {}^{11}\text{B})$ 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 $[\text{BH}_4]^-$ (**1**), B_2H_6 (**2**), B_4H_{10} (**3**), B_5H_9 (**4**), or $[\text{B}_2\text{H}_7]^-$ (**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 ${}^{11}\text{B}$ nuclei such as in $[\text{B}_6\text{H}_6]^{2-}$ (**11**), to fast dynamic processes such as in B_6H_{10} (**5**), $[\text{B}_5\text{H}_8]^-$ (**10**), $[\text{B}_6\text{H}_7]^-$ (**11-H**), $[\text{B}_3\text{H}_8]^-$ (**13**), $\text{Be}(\text{BH}_4)_2$ (**14**), $(\eta^5\text{-C}_5\text{H}_5)\text{BeBH}_4$ (**15**), $\text{Be}(\text{B}_3\text{H}_8)_2$ (**16**), $\text{Me}_2\text{AlB}_3\text{H}_8$ (**17**), or to instable species such as $[\text{B}_2\text{H}_6]^{2-}$ (**6**), B_2H_4 (**7**), B_3H_7 (**8**), and B_4H_8 (**9**). The experimental ${}^{11}\text{B}$ 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