Spin-Spin Coupling Constants $^1J(^{15}N,^{11}B)$ in Boron-Nitrogen Compounds. Experimental Data and DFT Calculations

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Boron-nitrogen compounds were studied with respect to indirect nuclear ^{15}N-^{11}B spin-spin coupling ($^1J(^{15}N,^{11}B)$). Some new experimental data were determined for aminoboranes and tetra-N-pyrrolylborate, and a variety of compounds with B-N single, double and triple bonds were examined using DFT methods for the calculation of $^1J(^{15}N,^{11}B)$ at the B3LYP/6-311+G(d,p) level of theory. The calculations predict magnitude and sign of $^1J(^{15}N,^{11}B)$ reasonably well, and the Fermi contact term was found to be dominant. A positive sign of $^1J(^{15}N,^{11}B)$ was calculated in the case of 1-aza-*closo*-dodecaborane(12), in contrast to all other compounds studied.

Key words: ^{15}N NMR, ^{11}B NMR, Boron-Nitrogen Compounds, Coupling Constants, DFT Calculations