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

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Boron-nitrogen compounds were studied with respect to indirect nuclear $^{15}\text{N}-^{11}\text{B}$ spin-spin coupling ($^{1}J(^{15}\text{N},^{11}\text{B})$). 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 $^{1}J(^{15}\text{N},^{11}\text{B})$ at the B3LYP/6-311+G(d,p) level of theory. The calculations predict magnitude and sign of $^{1}J(^{15}\text{N},^{11}\text{B})$ reasonably well, and the Fermi contact term was found to be dominant. A positive sign of $^{1}J(^{15}\text{N},^{11}\text{B})$ was calculated in the case of 1-aza-closo-dodecaborane(12), in contrast to all other compounds studied.

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