

Indirect Nuclear Spin-Spin Coupling Constants $^1J(^{17}\text{O}, ^{11}\text{B})$. First Observation and Calculation Using Density Functional Theory (DFT)

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Dedicated to Professor Dr. Max Herberhold on the occasion of his 70th birthday

Coupling constants $^1J(^{17}\text{O}, ^{11}\text{B})$ of borates, borane adducts and boranes with boron-oxygen bonds have been calculated on the basis of optimised molecular structures using the B3LYP/6-311+G(d,p) level of theory. This indicates that such coupling constants can be of either sign and that their magnitudes can be rather small. Since both ^{11}B and ^{17}O are quadrupole nuclei, it is therefore difficult to measure representative data. In the cases of trimethoxyborane and tetraethyldiboroxanes, it proved possible to obtain experimental data $^1J(^{17}\text{O}, ^{11}\text{B})$ (22 and 18 Hz) by measurement of ^{17}O NMR spectra at high temperature (120 °C and 160 °C) respectively. The magnitude of these coupling constants is in reasonable agreement with calculated data. In the case of the diboroxane, this points towards a bond angle B-O-B more close to 180° than to 140°.

Key words: Boranes, Borates, ^{17}O NMR, Coupling Constants, DFT Calculations