The Five-, Six- and Seven-Vertex Dicarbaboranes, Monocarbaborane Anions and Borane Dianions with *closo* Structures. Nuclear Spin-Spin Coupling Constants Calculated by DFT Methods

Bernd Wrackmeyer

Anorganische Chemie II, Universität Bayreuth, D-95440 Bayreuth, Germany

Reprint requests to Prof. Dr. B. Wrackmeyer. E-mail: b.wrack@uni-bayreuth.de

Z. Naturforsch. **60b,** 955 – 961 (2005); received June 13, 2005

Five-, six- and seven-vertex dicarbaboranes, carborane anions and borane dianions have been studied by DFT calculations at the B3LYP/6-311+G(d,p) level of theory, aiming at determining the indirect nuclear spin-spin coupling constants with an emphasis on $J(^{11}B,^{11}B)$, $J(^{13}C,^{11}B)$ and $J(^{13}C,^{13}C)$. The reasonable agreement with all experimental data suggests that the calculated data can be used in the discussion of the bonding situation in these cluster compounds, for which many coupling constants cannot be determined experimentally. The delocalisation of electron density is reflected by changes in both magnitude and sign of the coupling constants. The trend in the coupling constants between nuclei in antipodal positions points towards direct bonding interactions.

Key words: Boron Clusters, NMR, Coupling Signs, DFT Calculations