

# Theoretische und experimentelle Untersuchungen zur Protonierung substituierter *closo*-Hexaborate – $[\text{B}_6\text{H}_5\text{H}^{\text{fac}}\text{F}]^-$ und $[\text{B}_6\text{H}_5\text{H}^{\text{fac}}\text{CH}_3]^-$

Theoretical and Experimental Investigations on the Protonation of Substituted *closo*-Hexaborates –  $[\text{B}_6\text{H}_5\text{H}^{\text{fac}}\text{F}]^-$  and  $[\text{B}_6\text{H}_5\text{H}^{\text{fac}}\text{CH}_3]^-$

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Fluoro-hexahydro-*closo*-hexaborate(1-), Methyl-hexahydro-*closo*-hexaborate(1-), Protonation, NMR Data, Vibrational Spectra

The structural parameters and energies of the protonated compounds *closo*- $[\text{B}_6\text{H}_5\text{H}^{\text{fac}}\text{F}]^-$  and *closo*- $[\text{B}_6\text{H}_5\text{H}^{\text{fac}}\text{CH}_3]^-$  are calculated by MP2/6-31G\* optimization, as have the  $^1\text{H}$ ,  $^{11}\text{B}$ ,  $^{13}\text{C}$  and  $^{19}\text{F}$  NMR shifts using a tzp basis set and the RHF/GIAO method. The results for the octahedral molecule anions confirm the preferred localization of the additional proton in  $[\text{B}_6\text{H}_5\text{H}^{\text{fac}}\text{X}]^-$  in case of  $\text{X} = \text{CH}_3$  at the upper square pyramid topped by the *ipso*-boron atom, and in case of  $\text{X} = \text{F}$  at the lower one topped by the *antipodal* boron atom. The calculated NMR shifts are in good agreement with experimental data (this work). The higher BH frequencies observed for the protonated compounds as compared to the deprotonated parent clusters could be verified by *ab initio* frequency analyses.

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