Synthese, Spektren und Kristallstruktur von *cis*-Monobenzylmononitrotetrahydro-*closo*-hexaborat(2-)

Synthesis, Spectra and Crystal Structure of *cis*-Monobenzylmononitrotetrahydro-*closo*-hexaborate(2-)

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cis-Monobenzylmononitrotetrahydro-*closo*-hexaborate(2-), Crystal Structure, ^{11}B NMR Data, Vibrational Spectra

By electrochemical oxidation of (n-Bu_4N)[$B_6H_5H^{fac}(CH_2Ph)$] in the presence of nitrite ions in dichloromethane solution *cis*-$[B_6H_4(CH_2Ph)(NO_2)]^{2-}$ is formed. X-ray diffraction analysis has been performed on a single crystal of *cis*-$(Ph_4P)_2[B_6H_4(CH_2Ph)(NO_2)]\cdot H_2O\cdot CH_3CN$ (triclinic, space group P1; a = 11.338(5), b = 11.377(5), c = 21.081(5) Å, α = 93.727(5), β = 98.872(5), γ = 105.926(5)°, Z = 2). The ^{11}B NMR spectrum is consistent with a disubstituted octahedral B_6 cage with local C_{2v} symmetry. The IR and Raman spectra exhibit characteristic CH, NO_2, BN, BH and B_6 vibrations.