

Darstellung, spektroskopische Charakterisierung und Kristallstruktur von Dicyclopentadienylcobalt-hexahydro-*closo*-hexaborat



Synthesis, Spectroscopic Characterization and Crystal Structure of Dicyclopentadienylcobalt-hexahydro-*closo*-hexaborate $[(C_5H_5)Co(C_5H_4)B_6H_5H^{fac}]$

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Z. Naturforsch. **53 b**, 819–822 (1998); eingegangen am 9. April 1998

Dicyclopentadienylcobalt-hexahydro-*closo*-hexaborate, Crystal Structure, ^{11}B NMR

By reaction of $[B_6H_6H^{fac}]^-$ with cobaltocene in acetonitrile $[(C_5H_5)Co(C_5H_4)B_6H_5H^{fac}]$ is formed. Its crystal structure has been determined by single crystal X-ray diffraction analysis (monoclinic, space group $P2_1/n$ with $a = 9.786(2)$, $b = 9.726(2)$, $c = 13.938(2)$ Å, $\beta = 107.2850(3)^\circ$, $Z = 4$). The B_6 octahedron is slightly compressed in the direction of the B-C bond by about 1%, with B-B bond lengths between 1.69 and 1.87 Å. The ^{11}B NMR spectrum exhibits a 1:4:1 pattern of a monosubstituted B_6 cage. In the IR and Raman spectra characteristic B-H vibrations are observed.

* Sonderdruckanforderungen an Prof. Dr. W. Preetz.