

Darstellung, ^{11}B -NMR- und Schwingungsspektren von *cis*-Monoethylmononitrotetrahydro-*closo*-hexaborat(2-) sowie Kristallstruktur von *cis*-(Ph_4As) $_2$ [$\text{B}_6\text{H}_4(\text{C}_2\text{H}_5)(\text{NO}_2)$]

Synthesis, ^{11}B NMR and Vibrational Spectra of *cis*-Monoethylmononitrotetrahydro-*closo*-hexaborate(2-) and Crystal Structure of *cis*-(Ph_4As) $_2$ [$\text{B}_6\text{H}_4(\text{C}_2\text{H}_5)(\text{NO}_2)$]

C. Drewes und W. Preetz*

Institut für Anorganische Chemie der Christian-Albrechts-Universität,
Olshausenstr. 40, D-24098 Kiel

* Sonderdruckerfordernungen an Prof. Dr. W. Preetz. Fax: +49 431 880 1520.

Z. Naturforsch. **54 b**, 772–776 (1999); eingegangen am 26. Februar 1999

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

By electrochemical oxidation of (*n*- Bu_4N)[$\text{B}_6\text{H}_5\text{H}^{fac}(\text{C}_2\text{H}_5)$] in the presence of nitrite ions and of the base DBU in dichloromethane solution *cis*-[$\text{B}_6\text{H}_4(\text{C}_2\text{H}_5)(\text{NO}_2)$] $^{2-}$ is formed. X-ray diffraction analysis has been performed on a single crystal of *cis*-(Ph_4As) $_2$ [$\text{B}_6\text{H}_4(\text{C}_2\text{H}_5)(\text{NO}_2)$] (triclinic, space group $\text{P}\bar{1}$; $a = 10.673(4)$, $b = 10.907(4)$, $c = 21.237(4)$ Å, $\alpha = 80.789(4)$, $\beta = 83.117(4)$, $\gamma = 66.548(2)^\circ$, $Z = 2$). The ^{11}B NMR spectrum is consistent with a disubstituted octahedral B_6 cage with local C_s symmetry. The IR and Raman spectra exhibit characteristic CH_3 , CH_2 , NO_2 , BN , BH and B_6 vibrations.