

Kristallstruktur von $\text{Cs}_2[\text{B}_6\text{H}_5(\text{SCN})]$

Crystal Structure of $\text{Cs}_2[\text{B}_6\text{H}_5(\text{SCN})]$

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Z. Naturforsch. **53 b**, 816–818 (1998); eingegangen am 26. Januar 1998

Thiocyanato-pentahydro-*closo*-hexaborate(2-), Crystal Structure

By reaction of $[\text{B}_6\text{H}_6]^{2-}$ with $(\text{SCN})_2$ in dichloromethane at -80 C° the thiocyanatohexaborate anion is formed and can be isolated by ion exchange chromatography on diethylaminoethyl (DEAE) cellulose. The X-ray structure determination of $\text{Cs}_2[\text{B}_6\text{H}_5(\text{SCN})]$ (orthorhombic, space group *Pbca* with $a = 9.506(5)$, $b = 10.644(5)$, $c = 21.857(5)$ Å, $Z = 8$) reveals that the SCN substituent is bonded *via* the S atom with the B-S distance of 1.885(9) Å and the B-S-C angle of $99.8(5)^\circ$. The SCN group is nearly linear ($179.9(9)^\circ$).

* Sonderdruckanforderungen an Prof. Dr. W. Preetz.