Isoselenocyanatoborate - Kristallstrukturen von (n-Bu_4N)[$BH(NCSe)_3$] und (Ph_4P)[$B_3H_7(NCSe)$]

Isoselenocyanatoborates - Crystal Structures of (n-Bu_4N)[$BH(NCSe)_3$] and (Ph_4P)[$B_3H_7(NCSe)$]

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Triisoselenocyanatohydroborate(1-), Isoselenocyanato-heptahydrotriborate(1-), Crystal Structure

The treatment of $[B_6H_6]^{2-}$ with an excess of $(SCN)_2$ in dichloromethane in the presence of solid KOH gives the hexaisoselenocyanatodiborate anion $[B_2(NCSe)_6]^{2-}$ as an intermediate ($\delta(^{11}B) = -10.3$ ppm), from which $[BH(NCSe)_3]^-$ and elemental selenium are formed. The X-ray structure determinations on single crystals of (n-$Bu_4N)_2[BH(NCSe)_3]$ (**1**) (triclinic, space group P1 with $a = 8.512(2)$, $b = 10.885(3)$, $c = 14.895(4)$ Å, $\alpha = 79.52(2)$, $\beta = 74.86(2)$, $\gamma = 86.768(2)^\circ$, Z = 2) and (Ph_4P)[$B_3H_7(NCSe)$] (**2**) (monoclinic, space group C2, $a = 7.686(5)$, $b = 10.366(3)$, $c = 17.533(3)$ Å, $\beta = 108.89^\circ$, Z = 4) show that the selenocyanate groups are coordinated exclusively via the N atoms with average bond lengths of B-N = 1.52, C-N = 1.15, C-Se = 1.75 Å and angles N-C-Se = 179°, B-N-C = 168.7 - 176.8°. The N-B-N angles of **1** range from 107.5 to 109.5°.

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