Darstellung, ^{11}B- und ^{19}F-NMR-Spektren des Monofluoropentaiodo-*closo*-hexaboratanions sowie Kristallstruktur von $(CH_2Py_2)[B_6FI_5]$

Synthesis, ^{11}B and ^{19}F NMR Spectra of the Monofluoropentaiodo-*closo*-hexaborate Anion and the Crystal Structure of $(CH_2Py_2)[B_6FI_5]$

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Monofluoropentaiodo-*closo*-hexaborate(2-), Crystal Structure, ^{11}B and ^{19}F NMR Spectra

By reaction of *closo*-$[B_6H_5F]^{2-}$ in alkaline solution with excess iodine the monofluoropentaiodo-*closo*-hexaborate anion $[B_6FI_5]^{2-}$ is formed in good yield. The crystal structure of $(CH_2Py_2)[B_6FI_5]$ has been determined by single crystal X-ray diffraction analysis (orthorhombic, space group Pnma, a = 13.803(2), b = 11.759(2), c = 13.936(2) Å, Z = 4). The B-F-bond length is 1.41 Å, the B-I distances range from 2.13 to 2.17 Å, the B-B distances from 1.69 to 1.76 Å. According to the C_{4v} point symmetry the ^{11}B NMR spectrum of the anion exhibits three singlets at +3.8, –30.1 and –33.3 ppm with the intensity ratio 1:4:1, the ^{19}F NMR spectrum one quartet at -247.6 ppm with the coupling constant $^1J(^{19}F, ^{11}B)$ = 54 Hz.

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