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Selective synthesis of the $[2\text{-B}_{10}\text{H}_9\text{I}]^{2-}$ anion and some theoretical aspects of its iodination process.

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Abstract

New approaches to the selective synthesis of the $[2\text{-B}_{10}\text{H}_9\text{I}]^-$ anion have been reported based on careful control of the reaction medium acidity. The mechanism of the iodination was proposed and the regioselectivity of electrophilic substitution of the $[\text{B}_{10}\text{H}_{10}]^{2-}$ anion was explained based on B3LYP-calculations of the potential energy surface of the system using the mixed basis 6-31G*/LanL2DZ. The obtained compounds were characterized by IR and NMR (^1H and ^{11}B) spectroscopy, together with ESI-MS-spectrometry. The crystal structures of $(\text{PPh}_4)_2[2\text{-B}_{10}\text{H}_9\text{I}]$ and $\{(\text{PPh}_4)_2[2\text{-B}_{10}\text{H}_9\text{I}] \cdot 2\text{C}_4\text{H}_8\text{O}_2\}$ were determined by X-ray diffraction.

Keywords: *closo*-decaborate; iodination of boron clusters

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