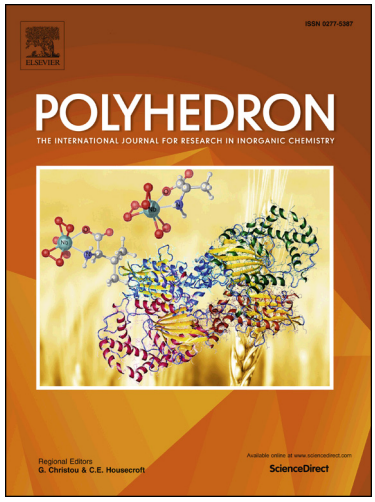

Selective synthesis of the $[2\text{-}B_{10}H_9I]^{2-}$ anion and some theoretical aspects of its iodination process.

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Selective synthesis of the $[2\text{-}B_{10}H_9I]^{2-}$ anion and some theoretical aspects of its iodination process.

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Abstract

New approaches to the selective synthesis of the $[2\text{-}B_{10}H_9I]^-$ 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 $[B_{10}H_{10}]^{2-}$ 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 $(PPh_4)_2[2\text{-}B_{10}H_9I]$ and $\{(PPh_4)_2[2\text{-}B_{10}H_9I]\cdot 2C_4H_8O_2\}$ were determined by X-ray diffraction.

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