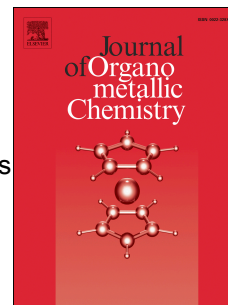


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Synthesis and selected properties of nonahalogenated 2-ammonio-decaborate anions and their derivatives substituted at N-centre

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Abstract

New preparative methods for halogenation of the cage producing the corresponding [2-NH₃-B₁₀X₉]⁻ species (**2**⁻ to **4**⁻, X= Cl, Br, I) have been developed using halogenations by elemental halogens in a glass pressure vessel. Compared to similar icosahedral species of formulation [1-H₃N-B₁₂X₁₁]⁻ (X= Cl, Br), the N-alkylation reactions in 10-vertex series proceed significantly more easily. The reason for this difference is conceivably due to the two orders of magnitude lower basicity of the amino group, with pK_a values in the interval from 9.27 to 8.37, and slightly lower steric strain around the reaction centre. Thus methylations with MeI under mild conditions provided the whole series of corresponding quarternary amines of the formulation [2-Me₃N-B₁₀X₉]⁻ (**5**⁻ to **7**⁻, X= Cl, Br, I). The effect of the steric strain of the surrounding halogens on the reactivity at the NH₃- centre could then be better seen from reactions with bulkier benzyl bromide. Under comparable conditions, these reactions resulted in the ready formation of disubstituted compounds in case of X= Cl (**8**⁻), mixture of mono and disubstituted derivatives for X= Br (**9**⁻, **10**⁻) or in monosubstituted product for X= I (**11**⁻) only. Dibenzyl derivative of the nonaiodinated products (**12**⁻) could be still obtained, however only under more forcing conditions. The single-crystal X-ray diffraction structures of all three polyhalogenated derivatives **2**⁻ to **4**⁻ are presented along with that for benzyl derivative **10**⁻, spectral and physicochemical properties of these polyhalogenated systems are outlined along with specific insights into specific properties of the NH₃ group.

Keywords: Boranes; Borate ions; Cluster; Halogenations; Electrochemistry; Capillary electrophoresis.

This paper is dedicated to Prof. Narayan S. Hosmane in the occasion of his 70th birthday and in recognition of his outstanding contributions to carborane and metallacarborane chemistries.

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