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Title:	Reactions of a BICAAC with hydroboranes: propensity for Lewis adduct formation and carbene insertion into the B–H bond†
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Keywords:	Bicyclic (alkyl)(amino) Carbene (BICAAC) Boranes
Issue Date:	2019
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Citation:	Dalton Transactions , 48(47), pp.17472 -17478.
Abstract:	The reactivity of a bicyclic (alkyl)(amino)carbene (BICAAC) towards different boranes has been examined in the present work. The reactions with boranes $BX_3 \cdot SME_2$ ($X = H, Cl, Br$), $BF_3 \cdot OEt_2$ and BCl_3 yield Lewis adducts $[BICAAC \cdot BH_3]$ (1), $[BICAAC \cdot BHCl_2]$ (2), $[BICAAC \cdot BH_2Cl]$ (3), $[BICAAC \cdot BF_3]$ (4), $[BICAAC \cdot BCl_3]$ (5) and $[BICAAC \cdot BBr_3]$ (6) respectively, whereas more hydridic boranes, 9-borabicyclo[3.3.1]nonane (9-BBN) and catecholborane (HBcat), enable the insertion of the carbene carbon into the B–H bond to form $[BICAAC(H)-(9-BBN)]$ (7) and $[BICAAC(H)-Bcat]$ (8). These complexes are the first examples of BICAAC–boron compounds and have been characterized using IR, multinuclear NMR spectroscopy, HRMS spectrometry and single crystal X-ray diffraction. Computational analyses were also performed to gain insight into the mechanism of B–H bond activation and adduct formation. Furthermore, the reactions of the BICAAC with boranes have been compared with the known reactions of CAACs and NHCs.
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