

Abstract

A modified version of CAACs named as bicyclic (alkyl)(amino) carbene (BICAAC) discovered by Bertrand and co-workers in 2017, have a great potential as a supporting ligand to the metal centers due to their better σ -donor and π -accepting properties as compared to NHCs and CAACs. Better σ -donor and π -accepting property of the carbene are well explored as small molecule activator and enthalpically strong bond activation such as Si-H, P-H and B-H. This property may also be exploited in transition as well as main group elements for stabilization of low valent elements. Given these facts, we have explored the chemistry of BICAAC with boranes ($\text{BH}_3\cdot\text{SMe}_2$), ($\text{BHCl}_2\cdot\text{SMe}_2$), ($\text{BH}_2\text{Cl}\cdot\text{SMe}_2$), (BCl_3) and ($\text{BBr}_3\cdot\text{SMe}_2$) to obtain their corresponding adducts, [BICAAC- BH_3] (**1**), [BICAAC- BHCl_2] (**2**), [BICAAC- BH_2Cl] (**3**), [BICAAC- BCl_3] (**4**) and [BICAAC- BBr_3] (**5**). Interestingly, BICAAC was reacted with 9-borabicyclo[3.3.1]nonane (9-BBN) and catecholborane (HBcat) that afforded the corresponding B-H activated complexes, [BICAAC(H)-9-BBN] (**6**) and [BICAAC(H)·Bcat] (**7**) as a consequence of B-H oxidative addition at the carbene carbon. Furthermore, the reactivity of adduct [BICAAC- BH_2Cl] (**3**) was explored for reduction reaction with potassium that afforded rare B-B bonded compound supported by two BICAAC units. All the adducts and B-B bonded compounds have been characterized by IR, multinuclear NMR and HRMS. Single crystal X-ray structure of the adducts and the B-B bonded compound have been well elucidated.