Title:	Well-Defined Ni(0) and Ni(II) Complexes of Bicyclic (Alkyl)(Amino)Carbene (MeBICAAC): Catalytic Activity and Mechanistic Insights in Negishi Cross-Coupling Reaction
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Abstract:	Negishi cross-coupling reaction of organozinc compounds as nucleophiles with aryl halides has drawn immense focus for C−C bond formation reactions. In comparison to the well-established library of Pd complexes, the C−C cross-coupling of this particular approach is largely primitive with nickel-complexes. Herein, we describe the syntheses of Ni(II) complexes, [(MeBICAAC)2NiX2] (X=Cl (1), Br (2), and I (3)) by employing the bicyclic (alkyl)(amino)carbene (MeBICAAC) ligand. The reduction of complexes 1–3 using KC8 afforded the two coordinate low valent, Ni(0) complex, [(MeBICAAC)2Ni(0)] (4). Complexes 1–4 have been characterized by spectroscopic techniques and their solid-state structures were also confirmed by X-ray crystallography. Furthermore, complexes 1–4 have been applied in a direct and convenient method to catalyze the Negishi cross-coupling reaction of various aryl halides with 2,6-difluorophenylzinc bromide or phenylzinc bromide as the coupling partner in the presence of 3 mol % catalyst. Comparatively, among all-pristine complexes, 1 exhibit high catalytic potential to afford value-added C−C coupled products without the use of any additive. The UV-vis studies and HRMS measurements of controlled stochiometric reactions vindicate the involvement of Ni(I)−NI(III) cycle featured with a penta-coordinated Ni(III)-aryl species as the key intermediate for 1 whereas Ni(0)/Ni(II) species are potentially involved in the catalytic cycle of 4.
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