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Title: Complexes of Palladium and Copper with Bicyclic (alkyl)(amino) Carbene (BICAAC)

Authors: Chakraborty, Soumyadeep (/jspui/browse?type=author&value=Chakraborty%2C+Soumyadeep)

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Abstract: Carbenes, neutral compounds containing divalent carbon atom with six electrons in valence shell, are the intriguing class of organic compound and possess potential to a new area of research particularly in organic transformations. After the successful isolation of N-heterocyclic carbene by Arduengo the major application of NHCs are found when they coordinate with transition metals. However, I have developed my interest on the advanced version of six-membered N-heterocyclic carbene namely bicyclic (alkyl)(amino) carbene, reported by Bertrand et al. which is more electrophilic (π -accepting) and nucleophilic (σ -donating) in comparison to NHCs. In the first chapter, the synthesis of a palladium complex stabilized by two bicyclic (alkyl)(amino) carbene units is demonstrated well $[(BICAAC)_2PdCl_2]$. The complex was synthesized starting from $PdCl_2$ reacting with the free carbene under inert conditions. The complex was fully characterized by M.P., NMR, single crystal and powder X-ray diffraction and high-resolution mass spectrometry. The $[(BICAAC)_2PdCl_2]$ complex has been investigated as a potential pre-catalyst towards different C-C coupling reactions (Heck-Mizoroki and Suzuki-Miyaura coupling) under the ambient condition with low catalyst loading. In the second chapter, the syntheses and photophysical studies of bicyclic (alkyl)(amino) carbene copper complex as $[(BICAAC)CuX]$ are demonstrated. The complexes were synthesized starting from CuX ($X = Cl, I$) with BICAAC. The mono and bis coordinated $Cu(I)$ complexes, $[(BICAAC)CuCl]$ and $[(BICAAC)_2Cu]^+[CuI_2]^-$, were characterized by NMR, single crystal X-ray diffraction and high-resolution mass spectrometry. The photophysical studies were also done in the solution phase. Then the neutral mononuclear copper complex $[(BICAAC)_2Cu]_0$ stabilized by two units of bicyclic (alkyl)(amino) carbene was attempted to synthesize starting from their carbene coordinated monohalide salt by potassium graphite (KC8) reduction method and was characterized by magnetic properties, absorption spectroscopy and HRMS of the complex.


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