

Abstract of Master's Thesis

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

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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 $[(\text{BICAAC})_2\text{PdCl}_2]$. 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 $[(\text{BICAAC})_2\text{PdCl}_2]$ 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 $[(\text{BICAAC})\text{CuX}]$ are demonstrated. The complexes were synthesized starting from CuX ($\text{X} = \text{Cl}, \text{I}$) with BICAAC. The mono and bis coordinated Cu(I) complexes, $[(\text{BICAAC})\text{CuCl}]$ and $[(\text{BICAAC})_2\text{Cu}]^+[\text{CuI}_2]^-$, 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 $[(\text{BICAAC})_2\text{Cu}]^0$ stabilized by two units of bicyclic (alkyl)(amino) carbene was attempted to synthesize starting from their carbene coordinated monohalide salt by potassium graphite (KC_8) reduction method and was characterized by magnetic properties, absorption spectroscopy and HRMS of the complex.