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Towards Isolation of Boron-containing *N*-Heterocyclic Carbene Complexes

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In 1991, Arduengo reported the isolation of *N*-heterocyclic carbene[1] (NHCs) as a stable free carbene. After that, NHCs have been employed in various complexes because of its strong σ donating ability, which can stabilize low-valent metal complex in catalytic cycles. Later, Bertrand et al. reported on the first cyclic alkyl(amino) carbenes (cAACs[2]) in which one of the N atoms of NHC is replaced by one σ-donating quaternary C atom. The π interaction of N atom decreases, which resulted in stronger π back bonding from metal. After that, various kind of NHCs derivatives have been reported in metal complexes.

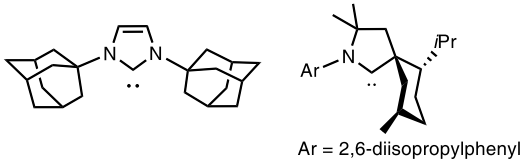

Figure 1. 1st Isolation of NHC and cAAC

In our previous work, we synthesized gold(I) diboron complex (**1**)[3], which activates isocyanide to form a gold\(I) complex bearing a 5-membered heterocyclic ring (**2**) (**Figure 2**). In this study, we focused on the structure of compound **(2**). Halide abstraction of compound(**2**) is expected to afford a complex(**3**) bearing a unique NHC in which one of the N atoms of NHC is replaced by π-accepting and electropositive B atom(**Figure 2**). This new ligand, if isolated, would be a 4-π antiaromatic system, which makes it a more π-accepting NHC ligand which encourages stronger π-back donation from metal centers than cAACs. However, our target complex has not been isolated so far. Recently, we tried new approaches towards isolation of our target complex. Firstly, we change the substituent of isocyanide which is less sterically hindered to avoid the destabilization by steric hinderance. Secondly, we will employ Group 9 and 10 metal centers that are better at π-back bonding to carbene to stabilize it(**Figure 4**). The strategy and attempt to isolate our target compound will be reported in the presentation.

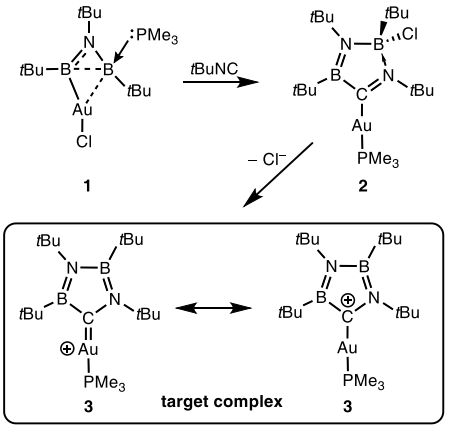

Figure 2. Previous work and synthesis of target complex

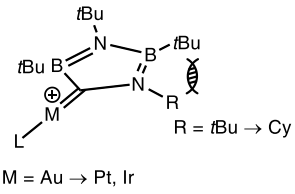

Figure 4. New design for stable carbene complexes

References

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[2] Lavallo, V.; Canac, Y.; Prasang, C.; Donnadieu, B.; Bertrand, G.; *Angew. Chem. Int. Ed.* **2005**, *44*, 5705−57

[3] Shang, R.; Saitou, S.; Jimenez-Halla, J. O.; Yamamoto, Y.; *Dalton Trans.*, **2018**,*47*, 5181–5188