Activation of sp^3 Carbon-Hydrogen Bonds Mediated by Bis(NHC) Iridium Complexes

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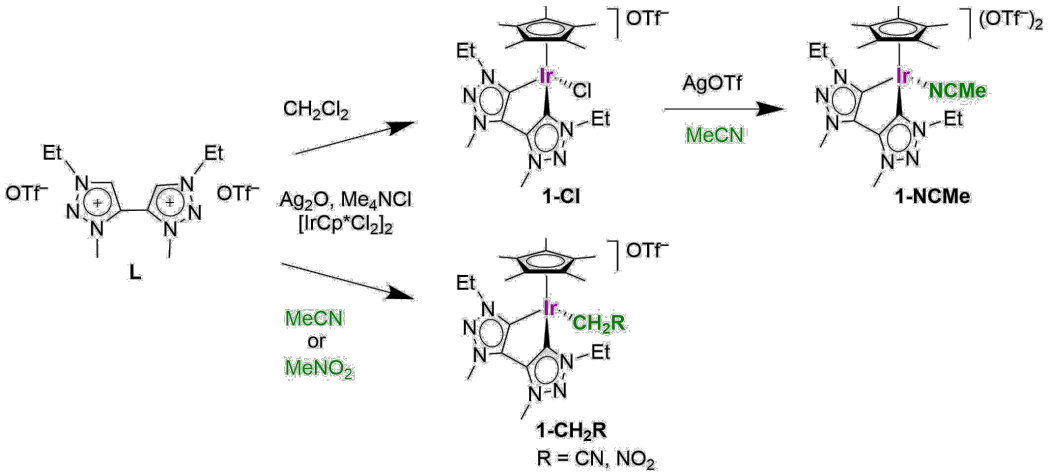
The activation and functionalization of C-H bonds remains a significant challenge for organometallic chemistry, with wide implications for organic synthesis. Many transition-metal systems that initiate stochiometric C-H activation are known, but complexes capable of both C-H activation and subsequent transformations of the substrate are relative rare,[1] especially for substrates with sp^3 C-H bonds.[2] Considering the high activity of iridium complexes in mediating C–H bond activation, in particular when bound to triazolylidene ligands,[3] we became interested in investigating a range of iridium complexes containing bis(carbene) ligands for facilitating alkyl C-H bond activation.[4]

Herein, we describe the C-H bond cleavage of acetonitrile and nitromethane by iridium(III) complexes bearing bis(triazolylidene) ligands. Metal hydroxide species formed during the metalation step have been demonstrated to be responsible of the bond scission.[5] Moreover, we will discuss opportunities to couple this alkyl fragment to substrates, potentially providing a new method for alkyl functionalization.



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