

IPr[#] Complexes—Highly-Hindered, Sterically-Bulky Cu(I) and Ag(I) N-Heterocyclic Carbenes: Synthesis, Characterization, and Reactivity

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Streszczenie

Metal–N-heterocyclic carbene (M–NHC) complexes are well-known as an important class of organometallic compounds widely used in transition-metal catalysis. Taking into account that the steric hindrance around the metal center is one of the major effects in M–NHC catalysis, the development of new, sterically hindered M–NHC complexes is an ongoing interest in this field of research. Herein, we report the synthesis and characterization of exceedingly sterically hindered, well-defined, air- and moisture-stable Cu(I) and Ag(I) complexes, [Cu(NHC)Cl] and [Ag(NHC)Cl], in the recently discovered IPr[#] family of ligands that hinge upon modular peralkylation of anilines. The complexes in both the BIAN and IPr families of ligands are reported. X-ray crystallographic analyses and computational studies were conducted to determine steric effects, Frontier molecular orbitals, and bond orders. The complexes were evaluated in the model hydroboration of the alkynes. We identified [Cu(BIAN–IPr[#])Cl] and [Ag(BIAN–IPr[#])Cl] as highly reactive catalysts with the reactivity outperforming the classical IPr and IPr*. Considering the attractive features of well-defined Cu(I)–NHC and Ag(I)–NHC complexes, this class of sterically bulky yet wingtip-flexible complexes will be of interest for catalytic processes in various areas of organic synthesis and catalysis.

Słowa kluczowe

Catalysts, Hydrocarbons, Ligands, Mathematical methods, Reactivity

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