

[Au(Np[#])Cl]: highly reactive and broadly applicable Au(I)–NHC catalysts for alkyne π -activation reactions

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Streszczenie

Cationic Au(I)–NHC (NHC = *N*-heterocyclic carbene) complexes have become an important class of catalysts for alkyne π -activation reactions in organic synthesis. In particular, these complexes are characterized by high stability of catalytic species engendered by strong σ -donation and metal backbonding. Herein, we report the synthesis and characterization of well-defined [Au(NHC)Cl] complexes featuring recently discovered IPr[#] family of ligands that hinge upon modular peralkylation of aniline. These ligands have been commercialized in collaboration with MilliporeSigma (IPr[#]: 915653; Np[#]: 915912; BIAN-IPr[#]: 916420). Evaluation of the [Au(NHC)Cl] complexes in a series of Au(I)–NHC-catalyzed π -functionalizations of alkynes, such as hydrocarboxylation, hydroamination and hydration, resulted in the identification of wingtip-flexible [Au(Np[#])Cl] as a highly reactive and broadly applicable catalyst with the re-activity outperforming the classical [Au(IPr)Cl] and [Au(IPr*)Cl] complexes. The utility of this catalyst has been demonstrated in the direct late-stage derivatization of complex pharmaceuticals. Structural and computational studies were conducted to determine steric effects, frontier molecular orbitals and bond orders of this class of catalysts. Considering the attractive features of well-defined Au(I)–NHC complexes, we anticipate that this class of bulky and wingtip-flexible Au(I)–NHCs based on the modular peralkylated naphthylamine scaffold will find broad application in π -functionalization of alkynes in various areas of organic synthesis and catalysis.

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