

[Ni(Np[#])(η^5 -Cp)Cl]: Flexible, Sterically Bulky, Well-Defined, Highly Reactive Complex for Nickel-Catalyzed Cross-Coupling

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Streszczenie

Ni–NHCs (NHC = *N*-heterocyclic carbene) have become an increasingly important class of complexes in catalysis and organometallic chemistry owing to the beneficial features of nickel as an abundant 3d metal. However, the development of well-defined and air-stable Ni–NHC complexes for cross-coupling has been more challenging than with Pd–NHC catalysis because of less defined reactivity trends of NHC ancillary ligands coordinated to Ni. Herein, we report the synthesis and catalytic activity of well-defined [Ni(NHC)(η^5 -Cp)Cl] complexes bearing the recently commercialized IPr[#] family of ligands (Sigma-Aldrich) and the versatile cyclopentadienyl throw-away ligand. The NHC ligands, IPr[#], Np[#], and BIAN-IPr[#], are prepared by robust and modular peralkylation of anilines. Most crucially, we identified [Ni(Np[#])(η^5 -Cp)Cl] as a highly reactive [Ni(NHC)(η^5 -Cp)Cl] complex, with the reactivity outperforming the classical [Ni(IPr)(η^5 -Cp)Cl] (IPr = 1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene). These [Ni(NHC)(η^5 -Cp)Cl] precatalysts were employed in the Suzuki–Miyaura and Kumada cross-coupling of aryl chlorides and aryl bromides. Computational studies were conducted to determine the steric effect and bond order analysis. Considering the attractive features of well-defined Ni–NHCs, we anticipate that this class of bulky and flexible Ni–NHC catalysts will find broad application in organic synthesis and catalysis.

Słowa kluczowe

Catalysis, Catalysts, Cross coupling reaction, Ligands, Reactivity

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