IPr*^{Oxa} – a new class of sterically-hindered, wingtip-flexible N,C-chelating oxazole-donor N-heterocyclic carbene ligands

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Streszczenie

N-heterocyclic carbenes (NHCs) have emerged as a major direction in ancillary ligand development for stabilization of reactive metal centers in inorganic and organometallic chemistry. In particular, wingtip-flexible NHCs have attracted significant attention due to their unique ability to provide a sterically-demanding environment for transition metals in various oxidation states. Herein, we report a new class of sterically-hindered, wingtip-flexible NHC ligands that feature N,C-chelating oxazole donors. These ligands are readily accessible through a modular arylation of oxazole derivatives. We report their synthesis and complete structural and electronic characterization. The evaluation of steric, electron-donating and π-accepting properties and coordination chemistry to Ag(I), Pd(II) and Rh(I) is described. Preliminary studies of catalytic activity in Ag, Pd and Rh-catalyzed coupling and hydrosilylation reactions are presented. This study establishes the fluxional behavior of a freely-rotatable oxazole unit, wherein the oxazolyl ring adjusts to the steric and electronic environment of the metal center. Considering the tremendous impact of sterically-hindered NHCs and their potential to stabilize reactive metals by N-chelation, we expect that this class of NHC ligands will be of broad interest in inorganic and organometallic chemistry.

Adres publiczny

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