

$\text{IPr}^{**}(4\text{-Bp})$ —Highly Hindered, Ring Extended N-Heterocyclic Carbenes

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Streszczenie

There is a strong demand for the development of sterically hindered N-heterocyclic carbenes due to their potential to stabilize reactive organometallic species. IPr^* ($\text{IPr}^* = 1,3\text{-bis}(2,6\text{-bis}(\text{diphenylmethyl})\text{-4-methylphenyl})\text{imidazo-2-ylidene}$) is a highly hindered and sterically flexible ligand, which has found broad utilization in coordination chemistry. Herein, we report the synthesis, structural, and electronic characterization of $\text{IPr}^{**}(4\text{-Bp})$ —a class of novel, sterically bulky, and easily accessible N-heterocyclic carbene ligands that bear biphenyl wingtips. Coordination chemistry to Ag(I) , Cu(I) , and Pd(II) is presented. The biphenyl wingtip permits extension of the $\%V_{\text{bur}}$ of $\text{IPr}^{**}(4\text{-Bp})$ to 58.8%, linear geometry, which is the highest reported to date for imidazol-2-ylidene ligands. The synthesis of an electron-rich congener, $\text{IPr}^{**\text{MeO}}(4\text{-Bp})$, which is analogous to the popular IPr^{MeO} ligand, is also presented. Coordination to Pd(II) demonstrates steric flexibility, where the $\%V_{\text{bur}}$ changes to 42.8% for square planar geometry. The study demonstrates that $\text{IPr}^{**}(4\text{-Bp})$ with an extended biphenyl wingtip is sterically bulkier than common imidazol-2-ylidenes, including IPr , IPr^* , $\text{IPr}^\#$, and $\text{IPr}^*(2\text{-Np})$. Considering the essential role of sterically hindered N-heterocyclic carbene ligands in various areas of coordination chemistry and metal catalysis, this new class of NHCs is poised for rapid and widespread application.

Słowa kluczowe

Aromatic compounds, Carbene compounds, Hydrocarbons, Ligands, Metals

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