Gold(I) Complexes of ImPyDippDipp and ImPyMesMes: Biaryl L-Shaped N-Heterocyclic Carbene Analogues of IPr and IMes

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Streszczenie

Imidazol-2-ylidenes, IPr and IMes, represent by far the most important and widely utilized N-heterocyclic carbenes in organic synthesis and catalysis. Herein, we report the synthesis, catalytic activity, and structural and electronic characterization of ImPyDippDipp and ImPyMesMes, sterically bulky and easily accessible biaryl L-shaped N-heterocyclic carbene analogues of IPr and IMes. These ligands exploit the rigid imidazo[1,5-*a*]pyridin-3-ylidene architecture to merge the properties of the biaryl scaffold with the electron-rich characteristics of the carbene center. The catalytic activity is evaluated in the gold(I)-catalyzed hydration of alkynes and cyclization N-propargylamides, two model reactions for π-activation of alkynes that have found broad application in organic synthesis. Structural and electronic evaluation indicates that biaryl L-shaped ImPyDippDipp and ImPyMesMes ligands are more sterically demanding and more electron σ-donating and π-accepting than the classical imidazol-2-ylidnes, IPr and IMes. Both of these L-shaped ligands show excellent catalytic activity in gold(I)-catalyzed hydration of alkynes and cyclization of N-propargylamides compared to their imidazol-2-ylidene congeners, IPr and IMes. Considering the tremendous impact of imidazol-2-ylidenes in homogeneous catalysis, we anticipate that this class of biaryl L-shaped NHCs will be rapidly and widely adopted to complement IPr and IMes N-heterocyclic carbenes.

Słowa kluczowe

Carbene compounds, Catalytic activity, Hydration,
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